

Planar $\mathcal{N} = 4$ Gauge Theory and the Hubbard Model

ADAM REJ^a, DIDINA SERBAN^{b,c} AND MATTHIAS STAUDACHER^{a,c}

*^aMax-Planck-Institut für Gravitationsphysik
Albert-Einstein-Institut
Am Mühlenberg 1, D-14476 Potsdam, Germany*

*^bService de Physique Théorique, CNRS-URA 2306
C.E.A.-Saclay
F-91191 Gif-sur-Yvette, France*

and

*^cKavli Institute for Theoretical Physics, University of California
Santa Barbara, CA 93106 USA*

Adam.Rej@aei.mpg.de, serban@spht.saclay cea.fr, matthias@aei.mpg.de

ABSTRACT

Recently it was established that a certain integrable *long-range* spin chain describes the dilatation operator of $\mathcal{N} = 4$ gauge theory in the $\mathfrak{su}(2)$ sector to at least three-loop order, while exhibiting BMN scaling to all orders in perturbation theory. Here we identify this spin chain as an approximation to an integrable *short-ranged* model of strongly correlated electrons: The Hubbard model.

1 Introduction

Recently it was discovered that the planar one-loop dilatation operator of supersymmetric $\mathcal{N} = 4$ gauge theory is completely integrable [1, 2]. This means that its spectrum may be exactly determined in the form of a set of non-linear Bethe equations. Evidence was found that this integrability is preserved beyond the one-loop approximation, and it was conjectured that the dilatation operator might be integrable to all orders in perturbation theory [3]. Given the usually benign, analytic nature of planar perturbation theory, one may then even hope for the theory's complete large N integrability at all values of the Yang-Mills coupling constant.

Deriving the dilatation operator from the field theory, and subsequently demonstrating its integrability, is not easy. The three-loop planar dilatation operator in the maximally compact $\mathfrak{su}(2|3)$ sector was found by Beisert, up to two unknown constants, by algebraic means in [4]. These constants could later be unequivocally fixed from the results of a solid field theory calculation of Eden, Jarczак and Sokatchev [5]. This basically completely determines the planar dilatation operator in this large sector up to three loops. Its restriction to $\mathfrak{su}(2)$ agrees with the original conjecture of [3]. Three-loop integrability in $\mathfrak{su}(2)$ was then demonstrated in [6] by embedding the dilatation operator into an integrable long-range spin chain due to Inozemtsev, and a three-loop Bethe ansatz was derived.

The Inozemtsev spin chain exhibited a four-loop breakdown of BMN scaling [8]. This scaling behavior seemed, and still seems, to be a desirable, albeit unproven, property of perturbative gauge theory. Mainly for that reason an alternative long-range spin chain, differing from the Inozemtsev model at and beyond four loops, was conjectured to exist in [7]. Its construction principles were an extension of the ones already laid out in [3]: (1) Structural consistency with general features of Yang-Mills perturbation theory, (2) perturbative integrability and (3) qualitative BMN scaling. The model's Hamiltonian is only known up to five loops, and increases exponentially in complexity with the loop order. In striking contrast, a very compact Bethe ansatz may be conjectured for the model and shown to diagonalize the Hamiltonian to the known, fifth, order. The conjecture reads

$$e^{ip_k L} = \prod_{\substack{j=1 \\ j \neq k}}^M \frac{u_k - u_j + i}{u_k - u_j - i}, \quad k = 1, \dots, M, \quad (1)$$

where the rapidities $u_k = u(p_k)$ are related to the momenta p_k through the expression

$$u(p_k) = \frac{1}{2} \cot \frac{p_k}{2} \sqrt{1 + 8g^2 \sin^2 \frac{p_k}{2}}, \quad (2)$$

and the energy should be given by

$$E(g) = -\frac{M}{g^2} + \frac{1}{g^2} \sum_{k=1}^M \sqrt{1 + 8g^2 \sin^2 \frac{p_k}{2}}. \quad (3)$$

This Bethe ansatz should yield the anomalous dimensions Δ of $\mathfrak{su}(2)$ operators of the

form

$$\text{Tr } X^M Z^{L-M} + \dots, \quad \text{where } \Delta(g) = L + g^2 E(g) \quad \text{with } g^2 = \frac{g_{\text{YM}}^2 N}{8\pi^2} = \frac{\lambda}{8\pi^2}. \quad (4)$$

The dots indicate all possible orderings of the partons Z and X inside the trace. This mixing problem is diagonalized by the spin chain Hamiltonian, where we interpret Z as an up-spin \uparrow and X as a down spin \downarrow . L is the length of the spin chain, and M the number of magnons \downarrow . These are the elementary excitations on the ferromagnetic vacuum state $|\uparrow\uparrow \dots \uparrow\uparrow\rangle$ which should be identified with the gauge theory's BPS state $\text{Tr } Z^L$. To leading one-loop order the spin chain Hamiltonian coincides with the famous isotropic nearest-neighbor Heisenberg XXX spin chain [1], and the corresponding Bethe ansatz is obtained by taking the $g \rightarrow 0$ limit of (1),(2),(3). See also [9] for a detailed explanation of the long range spin chain approach to gauge theory.

The higher-loop Bethe ansatz (1),(2),(3) has many intriguing properties [7], and it is suspicious that it should not have already appeared before in condensed matter theory. It is equally curious that the Hamiltonian should be so complicated, see [7], to the point that it is unknown how to write it down in closed form. Finally, and most importantly, the Bethe ansatz is expected to break down at wrapping order, i.e. it is *not* believed to yield the correct anomalous dimensions Δ starting from $\mathcal{O}(g^{2L})$. This suggests that the asymptotic Bethe ansatz (1),(2),(3) is actually not fully self-consistent at finite L and $g \neq 0$.

Nearly all work in solid state theory on the Heisenberg magnet has focused on the antiferromagnetic vacuum and its “physical” elementary excitations, the spinons. The only notable exceptions seem to be two articles of Sutherland and of Dhar and Shastry [10], where it was noticed that the dynamics of magnons in the ferromagnetic vacuum is far from trivial. This was later independently rediscovered and extended in the $\mathcal{N} = 4$ context in [1, 11]. In gauge theory the BPS vacuum is very natural, but it should be stressed that *all* states are important. In particular, it is interesting to ask what is the state of *highest* possible anomalous dimension. This is precisely the antiferromagnetic vacuum state, where $M = L/2$ and $E(g)$ in (3) should be maximized. Contrary to the BPS state $|\uparrow\uparrow \dots \uparrow\uparrow\rangle$ this state is highly nontrivial, as the Néel state $|\uparrow\downarrow\uparrow\downarrow \dots \uparrow\downarrow\rangle$ is not an eigenstate of the Heisenberg Hamiltonian. This problem was solved for $g = 0$ in the thermodynamic limit $L \rightarrow \infty$ in 1938 by Hulthén [12] using Bethe's ansatz.

Like the BPS state, the antiferromagnetic vacuum state is of very high symmetry. It should therefore also be of great interest in gauge theory. Let us then use the BDS Bethe ansatz (1),(2),(3) and compute the higher-loop corrections to Hulthén's solution. As the computation is done in the thermodynamic limit the BDS equations are perfectly reliable. The one-loop solution may be found in many textbooks. It is particularly well described in the lectures [14]. Adapting it to the deformed BDS case is completely straightforward. We will therefore mostly skip the derivation, referring to [14] for details, and immediately state the result for the energy of the antiferromagnetic vacuum:

$$E(0) = L \int_{-\infty}^{\infty} du \frac{\rho(u)}{u^2 + \frac{1}{4}} \quad \rightarrow \quad E(g) = L \int_{-\infty}^{\infty} du \rho(u) \left(\frac{i}{x^+(u)} - \frac{i}{x^-(u)} \right), \quad (5)$$

where the auxiliary spectral parameter x [7] is given by

$$x(u) = \frac{u}{2} \left(1 + \sqrt{1 - \frac{2g^2}{u^2}} \right), \quad \text{with} \quad x^\pm(u) = x(u \pm \frac{i}{2}). \quad (6)$$

Here $\rho(u)$ is the thermodynamic density of (magnon) excitations. It is found from solving the Bethe equations, which turn at $L \rightarrow \infty$ into a single non-singular integral equation for $\rho(u)$:

$$-\frac{dp(u)}{du} = 2\pi\rho(u) + 2 \int_{-\infty}^{\infty} du' \frac{\rho(u')}{(u-u')^2 + 1}, \quad (7)$$

where the derivative of the momentum density is, with $u_\pm = u \pm \frac{i}{2}$, given by

$$-\frac{dp(u)}{du} \Big|_{g=0} = \frac{1}{u^2 + \frac{1}{4}} \quad \rightarrow \quad i \frac{d}{du} \log \frac{x^+(u)}{x^-(u)} = \frac{i}{\sqrt{u_+^2 - 2g^2}} - \frac{i}{\sqrt{u_-^2 - 2g^2}}. \quad (8)$$

We notice that the r.h.s. of Hulthén's equation (7) does not depend explicitly on the coupling constant g (since the S-matrix of the BDS Bethe equation, i.e. the r.h.s. of (1) does not look different, in the u -variables, from the one of the Heisenberg model). Furthermore, the kernel of the integral equation is of difference form and the integration range is infinite. The equation may therefore immediately solved for $\rho(u)$, for all g , by Fourier transform:

$$\rho(u) \Big|_{g=0} = \frac{1}{2 \cosh \pi u} \quad \rightarrow \quad \rho(u) = \int_0^\infty \frac{dt}{2\pi} \frac{\cos(tu) J_0(\sqrt{2}gt)}{\cosh\left(\frac{t}{2}\right)}. \quad (9)$$

Plugging this result into the energy expression (5) one finds

$$E(0) = L 2 \log 2 \quad \rightarrow \quad E(g) = L \frac{4}{\sqrt{2}g} \int_0^\infty \frac{dt}{t} \frac{J_0(\sqrt{2}gt) J_1(\sqrt{2}gt)}{1 + e^t}, \quad (10)$$

where $J_0(t), J_1(t)$ are standard Bessel functions.

Now, it so turns out that the expressions for $\rho(u)$ in (9) and $E(g)$ in (10) are very famous results in the history of condensed matter theory. The latter is, up to an overall minus sign, identical to the ground state energy of the one-dimensional *Hubbard model* at half filling. It was shown to be integrable and solved by Bethe Ansatz in 1968 by Lieb and Wu [15]. Since then a very large literature on the subject has developed. For some good re- and overviews, see [16]. The Hubbard model is not quite a spin chain, but rather a model of N_0 itinerant electrons on a lattice of length L . The electrons are spin- $\frac{1}{2}$ particles. Due to Pauli's principle the possible states at a given lattice site are thus four-fold: (1) no electron, (2) one spin-up electron \uparrow , (3) one spin-down electron \downarrow , (4) two electrons of opposite spin $\uparrow\downarrow$. Hubbard's Hamiltonian reads, in one dimension

$$H_{\text{Hubbard}} = -t \sum_{i=1}^L \sum_{\sigma=\uparrow,\downarrow} \left(c_{i,\sigma}^\dagger c_{i+1,\sigma} + c_{i+1,\sigma}^\dagger c_{i,\sigma} \right) + tU \sum_{i=1}^L c_{i,\uparrow}^\dagger c_{i,\uparrow} c_{i,\downarrow}^\dagger c_{i,\downarrow}. \quad (11)$$

The operators $c_{i,\sigma}^\dagger$ and $c_{i,\sigma}$ are canonical Fermi operators satisfying the anticommutation relations

$$\begin{aligned} \{c_{i,\sigma}, c_{j,\tau}\} &= \{c_{i,\sigma}^\dagger, c_{j,\tau}^\dagger\} = 0, \\ \{c_{i,\sigma}, c_{j,\tau}^\dagger\} &= \delta_{ij} \delta_{\sigma\tau}. \end{aligned} \quad (12)$$

We see that the Hamiltonian consists of two terms, a kinetic nearest-neighbor hopping term with strength t , and an ultralocal interaction potential with coupling constant U . Depending on the sign of U , it leads to on-site attraction or repulsion if two electrons occupy the same site.

Comparing the BDS result (10) with the result of Lieb and Wu for the ground state energy of the half-filled band, where the number of electrons equals the number of lattice sites, i.e. $N_0 = L$, we see that the two energies coincide *exactly* under the identification

$$t = -\frac{1}{\sqrt{2}g} \quad U = \frac{\sqrt{2}}{g}. \quad (13)$$

This leads us to the conjecture that the BDS long-range spin chain, where, by construction, g is assumed to be small, is nothing but the strong coupling limit of the Hubbard model under the identification (13). In the following we will show that this is indeed the case, even away from the antiferromagnetic ground state. In fact, we shall demonstrate that it is *exactly true at finite L* up to $\mathcal{O}(g^{2L})$ where the BDS long-range chain loses its meaning. This will, however, require the resolution of certain subtleties concerning the boundary conditions of the Hamiltonian (11). As it stands, it will only properly diagonalize the BDS chain if the length L is odd. If the length is even, we have to subject the fermions to an Aharonov-Bohm type magnetic flux ϕ . The Hamiltonian in the presence of this flux remains integrable and reads

$$H = \frac{1}{\sqrt{2}g} \sum_{i=1}^L \sum_{\sigma=\uparrow,\downarrow} \left(e^{i\phi_\sigma} c_{i,\sigma}^\dagger c_{i+1,\sigma} + e^{-i\phi_\sigma} c_{i+1,\sigma}^\dagger c_{i,\sigma} \right) - \frac{1}{g^2} \sum_{i=1}^L c_{i,\uparrow}^\dagger c_{i,\uparrow} c_{i,\downarrow}^\dagger c_{i,\downarrow}, \quad (14)$$

where the twist is given by¹

$$\begin{aligned} \phi_\sigma &= \phi, \quad \sigma = \uparrow, \downarrow, \\ \phi &= 0 \text{ for } L = \text{odd} \quad \text{and} \quad \phi = \frac{\pi}{2L} \text{ for } L = \text{even}. \end{aligned} \quad (15)$$

An alternative way to introduce the Aharonov-Bohm flux is to perform a suitable gauge transformation and to thereby concentrate the magnetic potential on a single link, say the one connecting the L 'th and the first site. It is then clear that considering a non-zero flux amounts to considering twisted boundary conditions for the fermions.

The vacuum of the Hamiltonian (11) is the empty lattice of length L . Here the elementary excitations are up (\uparrow) and down (\downarrow) spins. Two electrons per site ($\downarrow\uparrow$) are

¹For odd L the twist ϕ_σ could alternatively be chosen as any integer multiple of $\frac{\pi}{L}$, while for even L any odd-integer multiple of $\frac{\pi}{2L}$ is possible. A compact notation which does not distinguish the cases L odd or even is $\phi = \frac{\pi(L+1)}{2L}$.

considered a bound state of elementary excitations. These constituents of the bound states are repulsive (as $g > 0$). For our purposes it is perhaps more natural to consider the BPS vacuum:

$$|Z^L\rangle = |\uparrow\uparrow \dots \uparrow\uparrow\rangle = c_{1\uparrow}^\dagger c_{2\uparrow}^\dagger \dots c_{L-1\uparrow}^\dagger c_{L\uparrow}^\dagger |0\rangle \quad (16)$$

We may then perform a particle-hole transformation on the up-spin electrons.

$$\circ \iff \uparrow \quad (17)$$

$$\downarrow \iff \updownarrow \quad (18)$$

Now single up-spins (\uparrow) are considered to be empty sites, while the elementary excitations are holes (\circ) and two electrons states (\updownarrow). In the condensed matter literature, such a transformation is often called a Shiba transformation and it is known to reverse the sign of the interaction. The standard Shiba transformation contains an alternating sign in the definition of the new creation/annihilation operators, designed to recover the hopping term, at least in the periodic case. The price to pay is that for odd lengths the sign of the hole hopping term will change on the link connecting the last (L 'th) and the first site. In other words, the particle/hole transformation introduces an extra flux of πL seen by holes. Since we prefer to distribute this twist uniformly along the chain, we remove the signs in the definition of the hole operators² and put

$$c_{i,\circ} = c_{i,\uparrow}^\dagger, \quad c_{i,\circ}^\dagger = c_{i,\uparrow}, \quad (19)$$

$$c_{i,\updownarrow} = c_{i,\downarrow}, \quad c_{i,\updownarrow}^\dagger = c_{i,\downarrow}^\dagger. \quad (20)$$

Under the particle/hole transformation, the charge changes sign and the corresponding hopping terms get complex conjugated. An extra minus sign comes from the reordering of the hole operators. Therefore we may write the Hamiltonian in its dual form

$$H = \frac{1}{\sqrt{2}g} \sum_{i=1}^L \sum_{\sigma=\circ,\updownarrow} \left(e^{i\phi_\sigma} c_{i,\sigma}^\dagger c_{i+1,\sigma} + e^{-i\phi_\sigma} c_{i+1,\sigma}^\dagger c_{i,\sigma} \right) - \frac{1}{g^2} \sum_{i=1}^L (1 - c_{i,\circ}^\dagger c_{i,\circ}) c_{i,\updownarrow}^\dagger c_{i,\updownarrow}. \quad (21)$$

where $\phi_\uparrow = \phi_\downarrow$, while $\phi_\circ = \pi - \phi_\uparrow$. $\phi_\uparrow = \phi_\downarrow = \phi$, multiple of $2\pi/L$, Comparing the two expressions (14) and (21) we conclude that under the duality transformation, the Hamiltonian (14) transforms as

$$H(g; \phi, \phi) \rightarrow -H(-g; \pi - \phi, \phi) - \frac{M}{g^2} \quad (22)$$

As predicted, the sign of the interaction changes upon dualization. The effect is that holes \circ and states with two electrons per site \updownarrow attract each other and form bound states \downarrow , the magnons.

²This amounts to a gauge transformation.

2 Effective Three-Loop Spin Hamiltonian

In this chapter we will explicitly demonstrate that the Hubbard Hamiltonian (11) generates at small g the three-loop dilatation operator of $\mathcal{N} = 4$ gauge theory in the $\mathfrak{su}(2)$ sector [3]. The BDS long-range spin Hamiltonian [7] is thus seen to emerge as an *effective* Hamiltonian from the underlying short-range system. Note that the small g limit, relevant to perturbative gauge theory, corresponds, via (13), to the *strong coupling* limit $U \rightarrow \infty$ of the Hubbard model in condensed matter parlance.

Our claim may be verified immediately to two-loop order, using well-known results in the literature. Klein and Seitz [17] proposed the strong-coupling expansion of the half-filled Hubbard model to $\mathcal{O}(g^7)$. The two-loop result $\mathcal{O}(g^4)$ was later confirmed by Takahashi [18]. In fact, eq. (2.15) of his paper³ precisely agrees with the two-loop piece of the BDS Hamiltonian (and therefore with two-loop gauge theory [3]) under the parameter identification (13). Eq. (2.15) of [18] also contains certain four-spin terms which only couple, since our system is one-dimensional, to a length $L = 4$ ring. These are a first manifestation of certain unwanted terms which we need to eliminate by appropriate boundary conditions and twisting, see (14),(15), to be discussed in more detail below.

When one now turns to the three-loop $\mathcal{O}(g^6)$ result of Klein and Seitz [17] as obtained in 1972, one unfortunately finds that their effective Hamiltonian disagrees with the BDS Hamiltonian at this order. We have been unable to find a later paper in the vast condensed matter literature on the subject which confirms or corrects their 33 year old calculation. We have therefore decided to check their computation in detail. And indeed we found a mistake, see below. Correcting it, we reproduce the planar three-loop $\mathfrak{su}(2)$ dilatation operator [3, 4, 5], see (28),(29) below.

For the remainder of this chapter it is convenient to use (11) and rewrite it (see Appendix A.3 for a discussion about the relevance of the twist factors in computing the effective Hamiltonian) in the form:

$$H_{\text{Hubbard}} = - \sum_{i < j}^L t_{ij} (X_{ij} + X_{ji}) + tU \sum_{i=1}^L c_{i,\uparrow}^\dagger c_{i,\uparrow} c_{i,\downarrow}^\dagger c_{i,\downarrow}. \quad (23)$$

where $X_{ij} = \sum_{\sigma=\uparrow,\downarrow} c_{i,\sigma}^\dagger c_{j,\sigma}$ and $t_{ij} = t \delta_{i+1,j}$.

2.1 Generalities

The Hamiltonian (23) consists of two parts: A *hopping term* involving the coefficients t_{ij} , and the *atomic part*. The latter is diagonalized by eigenstates describing localized electrons at sites x_i . The ground-state subspace \mathcal{E}_0 of the atomic part is spanned by $c_{1\tau_1}^\dagger c_{2\tau_2}^\dagger \cdots c_{L-1,\tau_{L-1}}^\dagger c_{L\tau_L}^\dagger |0\rangle$. Here we are interested in the limit of large U , with t staying relatively small. The atomic part tends to localize the electrons, while some hopping may still occur. At low temperatures this corresponds to small fluctuations around \mathcal{E}_0 states, since each hopping of the electron from one site to another is suppressed by a

³Incidentally, this is the famous paper where the next-nearest neighbor correlation function of the Heisenberg antiferromagnet was first obtained. We took this as a hint that the half-filled Hubbard model “knows” something about long-range deformations of the Heisenberg model.

factor of order of $1/U$. One can now pose the question whether it is possible, for large U and low temperature, to find an effective operator h acting in \mathcal{E}_0 whose eigenvalues

$$h|\phi\rangle = E|\phi\rangle \quad (24)$$

are the same as for the one of the Hamiltonian (11):

$$H|\psi\rangle = E|\psi\rangle. \quad (25)$$

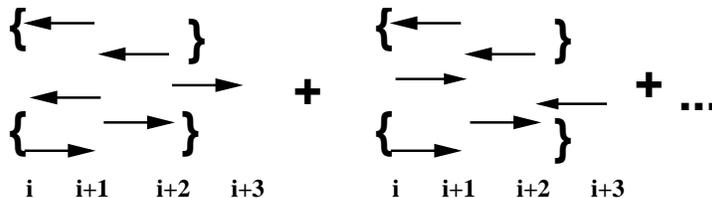
The answer is to the positive and has a long history [19]. A formal and rigorous treatment of this subject is presented in appendix A.

It is however instructive to discuss (24) in a more heuristic way. It is obvious that the effective Hamiltonian h must properly include the hopping effects. On the other hand it acts only in a subspace of the full state space, where configurations with double occupancies are projected out. This means that (24) should describe processes with *virtual* intermediate states, corresponding to electrons hopping from site i to site j and subsequently hopping back. Since every nearest-neighbor hopping is suppressed by $1/U$ it is clear that the $1/U$ expansion of h will result in increasingly long-range interactions. What kind of terms may appear in h ? A first guess leads to products of hopping operators X_{ij} with the condition that they will not move states out of the space \mathcal{E}_0 . Since X_{ij} annihilates an electron at site j and creates a new one at i , we see that only such products of X_{ij} operators are allowed which result in the same number of creation and annihilation operators at a given lattice site. Since each product of creation and annihilation operators may be represented in terms of $\mathfrak{su}(2)$ spin operators, we conclude that the effective Hamiltonian (24) must be of spin-chain form!

2.2 Three-Loop Result

We have used perturbation theory for degenerate systems (see appendix A.1, where also some details of the computation scheme are explained) to derive the effective Hamiltonian to three loops. The result up to sixth order (i.e. three loops) for the formal perturbation theory expansion is found in (89) in appendix A.2. It may be shown to be completely equivalent to the expansion obtained by Klein and Seitz in [17].

The formal expansion is then converted into a diagrammatic expansion, see again appendix A.2. We agree with Klein and Seitz with all perturbation theory diagrams up to sixth order as presented in their paper, except that we find that they missed a few diagrams (of type 'a' as in Fig 5. of their paper). These are the following diagrams (summation over i is understood):



where ... means arrow-reversed diagrams.

We have confirmed all diagram evaluations performed in [17], except for the contribution of the diagrams of type f in equation (C3) of the mentioned paper, where there is an overall factor of 16 missing. We believe this to be a typographical error. There is however also an additional contribution from the mentioned four diagrams which were not included in their computations. Explicit calculation shows, that the missing terms yield

$$-\left(\frac{1}{U}\right)^6 Ut(16A_1 - 4A_2 + 2B_3 - 2B_1 - 2B_2), \quad (26)$$

where

$$A_s = \sum_{i=1}^L (1 - \mathcal{P}_{i,i+s}), \quad B_1 = \sum_{i=1}^L (1 - \mathcal{P}_{i,i+1} \mathcal{P}_{i+2,i+3}),$$

$$B_2 = \sum_{i=1}^L (1 - \mathcal{P}_{i,i+2} \mathcal{P}_{i+1,i+3}), \quad B_3 = \sum_{i=1}^L (1 - \mathcal{P}_{i,i+3} \mathcal{P}_{i+1,i+2}),$$

and \mathcal{P} is a spin permutation operator. Correcting the result of Klein and Seitz we find

$$h = \left[-2\left(\frac{1}{U}\right)^2 + 8\left(\frac{1}{U}\right)^4 - 56\left(\frac{1}{U}\right)^6 \right] tU A_1 + \left[-2\left(\frac{1}{U}\right)^4 + 16\left(\frac{1}{U}\right)^6 \right] tU A_2 +$$

$$4\left(\frac{1}{U}\right)^6 tU (B_2 - B_3). \quad (27)$$

Upon putting $U = \frac{\sqrt{2}}{g}$, $t = -\frac{1}{\sqrt{2}g}$ and after some simple algebra one rewrites (27) in the form

$$h = \sum_{i=1}^L (h_2 + g^2 h_4 + g^4 h_6 + \dots), \quad (28)$$

with

$$h_2 = \frac{1}{2}(1 - \vec{\sigma}_i \vec{\sigma}_{i+1}),$$

$$h_4 = -(1 - \vec{\sigma}_i \vec{\sigma}_{i+1}) + \frac{1}{4}(1 - \vec{\sigma}_i \vec{\sigma}_{i+2}),$$

$$h_6 = \frac{15}{4}(1 - \vec{\sigma}_i \vec{\sigma}_{i+1}) - \frac{3}{2}(1 - \vec{\sigma}_i \vec{\sigma}_{i+2}) + \frac{1}{4}(1 - \vec{\sigma}_i \vec{\sigma}_{i+3})$$

$$- \frac{1}{8}(1 - \vec{\sigma}_i \vec{\sigma}_{i+3})(1 - \vec{\sigma}_{i+1} \vec{\sigma}_{i+2})$$

$$+ \frac{1}{8}(1 - \vec{\sigma}_i \vec{\sigma}_{i+2})(1 - \vec{\sigma}_{i+1} \vec{\sigma}_{i+3}). \quad (29)$$

This is indeed the correct planar three-loop dilatation operator in the $\mathfrak{su}(2)$ sector of $\mathcal{N} = 4$ gauge theory [3]. It is fascinating to see its emergence from an important and well-studied integrable model of condensed matter theory.

3 Lieb-Wu Equations

The Hamiltonian (11) was shown to be integrable and diagonalized by coordinate Bethe ansatz in [15]. For a pedagogical treatment see [16]. This required finding the dispersion relation of the elementary excitations \uparrow and \downarrow and working out their two-body S-matrix. It is indeed a *matrix* since there are two types of excitations, hence their ordering matters. The scattering of two up- or two down-spins is absent, as identical fermions behave like free particles. The scattering of different types of fermions is non-trivial due to their on-site interaction. After working out the S-matrix one needs to diagonalize the multi-particle system by a *nested* Bethe ansatz. The result of this procedure, generalized to the case with magnetic flux, yields the Lieb-Wu equations:

$$e^{i\tilde{q}_n L} = \prod_{j=1}^M \frac{u_j - \sqrt{2}g \sin(\tilde{q}_n + \phi) - i/2}{u_j - \sqrt{2}g \sin(\tilde{q}_n + \phi) + i/2}, \quad n = 1, \dots, L \quad (30)$$

$$\prod_{n=1}^L \frac{u_k - \sqrt{2}g \sin(\tilde{q}_n + \phi) + i/2}{u_k - \sqrt{2}g \sin(\tilde{q}_n + \phi) - i/2} = \prod_{\substack{j=1 \\ j \neq k}}^M \frac{u_k - u_j + i}{u_k - u_j - i}, \quad k = 1, \dots, M \quad (31)$$

where the twist is given⁴ in (15) and the energy is

$$E = \frac{\sqrt{2}}{g} \sum_{n=1}^L \cos(\tilde{q}_n + \phi). \quad (32)$$

Here we have already specialized to the half-filled case with $N_0 = L$ fermions and $M \leq L/2$ down-spin fermions (there are thus $L - M$ up-spin fermions in the system).

This form of the Hubbard model's Bethe equations is very convenient for demonstrating rather quickly that the $g \rightarrow 0$ limit yields the spectrum of the Heisenberg magnet. In fact, the Lieb-Wu equations decouple at leading order and become

$$e^{i\tilde{q}_n L} = \prod_{j=1}^M \frac{u_j - i/2}{u_j + i/2} \left(1 + \mathcal{O}(g)\right), \quad n = 1, \dots, L \quad (33)$$

$$\left(\frac{u_k + i/2}{u_k - i/2}\right)^L = \prod_{\substack{j=1 \\ j \neq k}}^M \frac{u_k - u_j + i}{u_k - u_j - i}, \quad k = 1, \dots, M \quad (34)$$

Eqs. (34) are already identical to the ones of the Heisenberg magnet (see e.g. [1],[14]). The r.h.s. of (33) is, to leading order $\mathcal{O}(g^0)$, the eigenvalue of the shift operator of the chain (again, [1],[14]). In gauge theory we project onto cyclic states, so we may take the eigenvalue to be one, and solve immediately for the L momenta \tilde{q}_n to leading order:

$$e^{i\tilde{q}_n L} = 1 \quad \implies \quad \tilde{q}_n = \frac{2\pi}{L}(n - 1) + \mathcal{O}(g), \quad n = 1, \dots, L. \quad (35)$$

⁴The Lieb-Wu equations for arbitrary twist are given in appendix C.

But now we have to find the energy. Plugging the result (35) into the expression (32) conveniently eliminates the spurious $\mathcal{O}(1/g)$ term in the energy. We therefore need to find the $\mathcal{O}(g)$ corrections to the momenta in (35) from (30). Luckily, this is a *linear* problem; solving it one computes the $\mathcal{O}(g^0)$ term of (32) as

$$E = \sum_{k=1}^M \frac{1}{u_k^2 + \frac{1}{4}} + \mathcal{O}(g), \quad (36)$$

which is the correct expression for the energy of the Heisenberg magnet.

The starting point for the small g expansion of the Lieb-Wu equations are therefore Bethe's original equations (34),(36) in conjunction with the free particle momentum condition (35). It is interesting that all non-linearities are residing in the one-loop Bethe equations (34). Once these are solved for a given state, the perturbative expansion is obtained from a linear, recursive procedure. It allows for efficient and fast numerical computation of the loop corrections to any state once the one-loop solution is known. A simple tool for doing this with e.g. *Mathematica* may be found in Appendix B, along with a similar tool for the perturbative evaluation of the BDS equations.

We have applied this perturbative procedure to all⁵ (cyclic) states of the BDS chain as recorded, up to five loops, in Table 1, p.30 of [7]. The (twisted) Lieb-Wu equations (30),(31),(32) perfectly reproduce the energies of this table.

We found that that our version of the Hubbard model *precisely agrees* in all investigated cases with the results of the BDS ansatz up to and including the $(L - 1)$ -th loop order. On the other hand, invariably, at and beyond L 'th order of perturbation theory (corresponding to the $\mathcal{O}(g^{2L-2})$ terms in the energy E) the predictions of the two ansätze *differ*. See chapter 5 for some concrete examples.

It is also interesting to record the effects of the twists on the perturbative spectrum. A first guess might be that they should only influence the spectrum at and beyond wrapping order $\mathcal{O}(g^{2L-2})$, when the order of the effective interactions reaches the size of the ring, and the system should become sensitive to the boundary conditions. In actual fact, however, one finds that the twists generically influence the spectrum starting at already $\mathcal{O}(g^{L-2})$. This is the phenomenon of *demi-wrappings*. The Hubbard model at small g behaves effectively as a long-range spin chain due to the virtual "off-shell" decomposition of the magnon bound states \downarrow (which are sites occupied by a down-spin but no up-spin) into holes \circ (empty sites) and double-occupied sites \uparrow . The power of the coupling constant g counts the number of steps a hole \circ or \uparrow -particle is exercising during its virtual excursion, see also the discussion in section 2.1. We now observe that starting from at $\mathcal{O}(g^{L-2})$ the excitations \circ, \uparrow can (virtually) travel around the ring, and the amplitudes start to depend on the boundary conditions! A similar distinction between wrappings and demi-wrappings was qualitatively discussed in a recent paper on this subject [21]. Our procedure of twisting eliminates the demi-wrappings. Interestingly, this seems to leave no further freedom at and beyond wrapping order, at least in the context of our current construction.

The Lieb-Wu equations in the form (30),(31),(32) are very useful for the analysis of chains of small length. They are far less convenient in or near thermodynamic situations,

⁵The only exception are certain singular three-magnon states which require a special treatment.

i.e. when $L \rightarrow \infty$. The reason is the large number of momenta \tilde{q}_n one has to deal with. In (21) we have written a dual form of the Hamiltonian (14). Accordingly, we may write down the corresponding set of *dual* Lieb-Wu equations:

$$e^{iq_n L} = \prod_{j=1}^M \frac{u_j - \sqrt{2}g \sin(q_n - \phi) - i/2}{u_j - \sqrt{2}g \sin(q_n - \phi) + i/2}, \quad n = 1, \dots, 2M \quad (37)$$

$$\prod_{n=1}^{2M} \frac{u_k - \sqrt{2}g \sin(q_n - \phi) + i/2}{u_k - \sqrt{2}g \sin(q_n - \phi) - i/2} = - \prod_{\substack{j=1 \\ j \neq k}}^M \frac{u_k - u_j + i}{u_k - u_j - i}, \quad k = 1, \dots, M \quad (38)$$

where the energy is now given by

$$E = -\frac{M}{g^2} - \frac{\sqrt{2}}{g} \sum_{n=1}^{2M} \cos(q_n - \phi). \quad (39)$$

Again, we have specialized to the case of half-filling. A particular feature of the dual Hamiltonian (21) is that the twist is different for the two components. We are therefore led to use the Lieb-Wu equations for generic twist which are written down in Appendix C. This explains the minus sign in the right hand of (38), $e^{i(\phi_1 - \phi_0)} = e^{i(2\phi - \pi)L} = -1$. Note that $\phi \rightarrow -\phi$ is a symmetry of the equations (but not of the solutions), as we may change $u \rightarrow -u$ and $q \rightarrow -q$. Note also that therefore the set of $L + 2M$ momenta $(\tilde{q}_n, -q_n)$ corresponds to the $L + 2M$ solutions of the first Lieb-Wu equation (30).

4 Magnons from Fermions

In chapter 2 we proved, to three-loop order, that the Hamiltonian of the BDS long-range spin chain emerges at weak coupling g from the twisted Hubbard Hamiltonian as an effective theory. Pushing this proof to higher orders would be possible but rather tedious. Note, however, that the BDS Hamiltonian is, at any rate, only known to five-loop order [7]. What we are really interested in is whether the Bethe ansatz (1),(2),(3), which was *conjectured* in [7], may be *derived* from the Bethe equations of the Hubbard model, i.e. from the Lieb-Wu equations of the previous chapter. We will now show that this is indeed the case. The derivation will first focus on a single magnon (section 4.1), where it will be shown that the magnons \downarrow of the long-range spin chain are bound states of holes \circ and double-occupations \uparrow , as is already suggested by the perturbative picture of chapter 2. It will culminate in 4.3, where we demonstrate that the bound states alias magnons indeed scatter according to the r.h.s. of (1). An alternative proof may be found in appendix E.

Unlike the BDS long-range spin chain, the twisted Hubbard model is well-defined away from weak coupling, and actually for arbitrary values of g . An important question is whether the twisted Hubbard model allows to explain the vexing discrepancies between gauge and string theory [22, 6]. Unfortunately this does not seem to be the case. We have carefully studied the spectrum of two magnons in section 4.2, and find that their is no order of limits problem as the coupling g and the length L tend to infinity while

g/L stays finite. The scattering phase shift indeed always equals the one predicted by the BDS chain.

The Hubbard model contains also many states which are separated at weak coupling by a large *negative* energy gap $\mathcal{O}(-1/g^2)$ from the magnons. This may be seen from the expression (39). For solutions with real momenta q_n the cosine is bounded in magnitude by one, and the constant part $-M/g^2$ cannot be compensated. These states are composed of, or contain, holes \circ and double-occupations \uparrow which are unconfined, i.e. which do not form bound states. Their meaning will need to be understood if it turns out that the $\mathcal{N} = 4$ gauge theory's dilatation operator can indeed be described by a Hubbard model beyond the perturbative three-loop approximation. In fact, it is clear from the expression for the anomalous dimension $\Delta = L + g^2 E(g)$ in (4) that each unconfined pair (\circ, \uparrow) shifts the classical dimension and thus the length down by one: $L \rightarrow L - 1$. Is this a first hint that the perturbative $\mathfrak{su}(2)$ sector of $\mathcal{N} = 4$ gauge theory does not stay closed at strong coupling, as was argued in [23]?

4.1 One-Magnon Problem

Let us then begin by studying the case of $M = 1$ down spin and $L - 1$ up spins, see [16],[24]. Clearly it is easiest to use the dual form of the Lieb-Wu equations (37),(38),(39). In the weakly coupled spin chain we have only L states, while in the Hubbard model we have L^2 states. This is because one down spin \downarrow is composed of one hole \circ and one double-occupation \uparrow . If we project to cyclic states, as in gauge theory, only one of the L states survives, namely the zero-energy BPS state. However, in order to derive the magnon dispersion law, we will not employ the projection for the moment. This way the magnon can carry non-zero momentum and energy. In the Hubbard model the magnon should be a $\circ\text{-}\uparrow$ bound state, and we therefore make the ansatz (with $\beta > 0$ and $q > 0$):

$$q_1 - \phi = \frac{\pi}{2} + q + i\beta, \quad q_2 - \phi = \frac{\pi}{2} + q - i\beta. \quad (40)$$

Here q_1 and q_2 are the quasimomenta of the \circ and the \uparrow particles. They are complex, where the imaginary part β describes the binding. Adding the real parts gives the momentum $2q$ of the magnon. The dual Lieb-Wu equations for one magnon, where we only have a single rapidity u , read

$$e^{iq_1 L} = \frac{u - \sqrt{2}g \sin(q_1 - \phi) - i/2}{u - \sqrt{2}g \sin(q_1 - \phi) + i/2}, \quad e^{iq_2 L} = \frac{u - \sqrt{2}g \sin(q_2 - \phi) - i/2}{u - \sqrt{2}g \sin(q_2 - \phi) + i/2}, \quad (41)$$

$$\frac{u - \sqrt{2}g \sin(q_1 - \phi) + i/2}{u - \sqrt{2}g \sin(q_1 - \phi) - i/2} \frac{u - \sqrt{2}g \sin(q_2 - \phi) + i/2}{u - \sqrt{2}g \sin(q_2 - \phi) - i/2} = -1. \quad (42)$$

By multiplying, respectively, the left and right sides of the two equations in (41) and using (40),(42) we derive

$$e^{i2qL} = 1 \quad \Rightarrow \quad q = \frac{\pi}{L} n \quad (n = 0, 1, \dots, L - 1). \quad (43)$$

This is just the statement that the magnon is free (there is nothing to scatter from) and its momentum $p := 2q$ is quantized on the ring of length L . Furthermore we can rewrite

(41) as

$$\sqrt{2} g \sin(q_{1,2} - \phi) - u = \frac{1}{2} \cot\left(\frac{q_{1,2} L}{2}\right). \quad (44)$$

Decomposing into real and imaginary parts we find, using the twist (15),

$$\sinh(\beta) = \frac{1}{2\sqrt{2}g} \frac{1}{\sin(q)} \tanh(\beta L), \quad (45)$$

and⁶

$$u = \sqrt{2}g \cos(q) \cosh(\beta) + \frac{(-1)^n (-1)^{\frac{L+1}{2}}}{2 \cosh(\beta L)}. \quad (46)$$

By analyzing (45) we may now discuss the existence of bound states. We see that for large L , where $\tanh(\beta L) \rightarrow 1$, we have, for given mode number n , exactly one⁷ solution with $\beta > 0$ for *all values of* $g > 0$. We also see that there is only one way to take the thermodynamic limit, independent of g :

$$\sinh(\beta) \simeq \frac{1}{2\sqrt{2}\pi} \frac{1}{ng/L}. \quad (47)$$

But this means that there is also only one way to take the BMN scaling limit, where $g, L \rightarrow \infty$ with g/L kept finite.

Let us then work out the energy of the magnon with momentum $p = 2q$. The exponential terms $\tanh(\beta L) \simeq 1 - 2e^{-2\beta L}$ may clearly be neglected at large L for arbitrary values of g , and we immediately find the dispersion law

$$E = -\frac{1}{g^2} + \frac{2\sqrt{2}}{g} \sin\left(\frac{p}{2}\right) \cosh(\beta) = -\frac{1}{g^2} + \frac{1}{g^2} \sqrt{1 + 8g^2 \sin^2 \frac{p}{2}}, \quad (48)$$

which is exactly the BDS result (3)! Likewise, again dropping the exponential terms from the rapidity relation (46), we find the BDS result (2) for the dependence of the rapidity $u(p)$ on the momentum $p_k = p = 2q$.

Note that our derivation only assumed the thermodynamic limit; it did *not* assume weak coupling. If the coupling g is weak we may in addition deduce from (45) that the binding amplitude β diverges logarithmically as $\beta \simeq -\log g$. We may then deduce that the exponential terms we dropped are

$$e^{-2\beta L} \simeq g^{2L}, \quad (49)$$

and therefore should be interpreted as $\mathcal{O}(g^{2L})$ wrapping corrections.

We just showed that L of the L^2 states of the Hubbard model's $M = 1$ states can be interpreted as magnons. The remaining $L(L - 1)$ states should correspond to solutions

⁶The sign of the second term in (46) may be changed by choosing a different gauge for the twist. This type of gauge dependence should not appear in physical observables such as the energy.

⁷Actually, if g becomes of the order of L such that g/L is larger than a certain threshold value, the bound state is lost. An additional real solution, c.f. appendix D, will appear.

where the momenta q_1, q_2 are *real*, i.e. these are not bound states. Among these, $L - 1$ states are cyclic. The unbound states are found as follows. We make the ansatz

$$q_1 - \phi = \frac{\pi}{2} + q + b, \quad q_2 - \phi = \frac{\pi}{2} + q - b, \quad (50)$$

which is completely general except for the assumption that q and b are *real*. The twisted dual Lieb-Wu equations (41),(42) still apply, and, using the same multiplication trick as before we find again (43). This is merely the statement that the total momentum is quantized on the ring of length L . The Lieb-Wu equations (41) now read

$$\sqrt{2} g \cos(q \pm b) - u = \frac{1}{2} \cot \left((q \pm b + \frac{\pi}{2} + \phi) \frac{L}{2} \right). \quad (51)$$

Let us first consider the unconfined *cyclic* states, i.e. the case of mode number $n = 0$ in (43), hence $q = 0$. We can then immediately find the energy of such states to-be from (39)

$$E = -\frac{1}{g^2}, \quad (52)$$

which is seen to not depend on b . But can we really find values for b which satisfy the Lieb-Wu equations (51)? How many solutions of this type do we have? The answer is easily found from subtracting either side of the two equations in (51). This yields the consistency condition

$$\frac{1}{2} \cot \left((\frac{\pi}{2} + \phi + b) \frac{L}{2} \right) = \frac{1}{2} \cot \left((\frac{\pi}{2} + \phi - b) \frac{L}{2} \right). \quad (53)$$

Now it is very easy to show that there are *precisely* $L - 1$ solutions of this equation:

$$b = \frac{\pi}{L} m \quad \text{with} \quad m = 1, \dots, L - 1. \quad (54)$$

Therefore, the $M = 1$ cyclic unconfined ($L - 1$ -fold degenerate) states resemble zero-energy ‘‘BPS states’’ with exact scaling dimension $\Delta = L - 1$. However, see appendix D.

Finally, let us study the number of states and the dispersion law of the unconfined states carrying non-zero total momentum $p = 2q = \frac{2\pi}{L} n$, cf. (43). We find that by eliminating u from (51) that

$$\sin(b) = \frac{1}{2\sqrt{2}g} \frac{1}{\sin(q)} \tan(bL), \quad (55)$$

which turns out to just be the analytic continuation of (45). It is not hard to prove that there are indeed generically $L - 1$ solutions for each value of the $L - 1$ non-zero values of q . This yields $(L - 1)^2$ states. Therefore, adding these to the $L - 1$ cyclic real solutions, and the L bound states, we have accounted for all of the L^2 states of the $M = 1$ problem. In appendix D we investigate the energy of the real solutions in the large g and large L limit. In the limit $L \rightarrow \infty$, the solutions of (55) become dense on the interval $(0, 2\pi)$, so

for any value of the magnon momentum $p = 2q$ we have a continuum of states, whose energies vary continuously. It is not clear how one would interpret these states in the context of the gauge theory, or, more generally, the AdS/CFT correspondence. It is possible that we need a model encompassing all the sectors of the gauge theory to be able to draw some conclusion about the large g limit.

Let us now turn to the mutual scattering of our magnons; first for two, and then for arbitrarily many. We shall find that the scattering is, up to exponential terms, indeed given by the r.h.s. of (1).

4.2 Two-Magnon Problem

The result of the previous section does not bode well for the hope expressed in the last chapter of [7] that wrapping might explain the discrepancies between gauge and string theory. This would require an order of limits problem as one takes the coupling g and the length L large. It is certainly not seen on the level of bound state formation, recall (45). However, one might still hope that the magnons constructed in the last section might somehow scatter in distinct ways at weak and strong coupling. By considering the $M = 2$ two-magnon problem we will now show that, unfortunately, this is not the case. It therefore seems that the AFS string Bethe ansatz [25] cannot be obtained from the twisted Hubbard model, at least not in the current version.

We proceed much as before, making the appropriate ansatz for two holes and two double-occupancies (with $\beta > 0$ and $q > 0$) bound into two magnons with momenta $p = 2q$ and $-p = -2q$:

$$\begin{aligned} q_1 - \phi &= \frac{\pi}{2} + q + i\beta, & q_3 - \phi &= \frac{\pi}{2} + q - i\beta, \\ q_2 - \phi &= -\frac{\pi}{2} - q + i\beta, & q_4 - \phi &= -\frac{\pi}{2} - q - i\beta. \end{aligned} \quad (56)$$

We derive (for simplicity assume $L \equiv 1 \pmod{4}$, which allows to assume that the two rapidities obey $u_1 = -u_2$) from the dual Lieb-Wu equations

$$\sinh(\beta) = \frac{\cosh(\beta) \cot(q) \sinh(\beta L)}{2\sqrt{2}g \cos(q) \cosh(\beta) (\cosh(\beta L) + \sin(qL)) - \cos(qL)}. \quad (57)$$

While looking superficially different, this agrees precisely, up to exponential terms, in the $L \rightarrow \infty$ limit with (45). It is crucial to note that, as in the previous $M = 1$ case, there is only *one* way to take the BMN scaling limit, which yields again (47). Likewise, we find, up to exponential corrections, for the rapidity

$$u^2 = \frac{1}{4} + g^2 + g^2 \cos(2q) \cosh(2\beta) = -\frac{1}{4} + g^2(\cos(2q) + \cosh(2\beta)). \quad (58)$$

Unfortunately one may now derive from (57) and (58) that the phase shift when the two magnons scatter at large L is always as in the BDS chain, and thus as in the gauge theory's near-BMN limit. The exponential corrections disappear in and near the BMN limit.

4.3 Many Magnons and a Proof of the BDS Formula

We have seen above that magnons \downarrow can arise as bound states of holes \circ and doubly occupied sites \uparrow . The solutions associated to these bound states are known in the condensed matter literature as k - Λ strings⁸ and were first considered by Takahashi⁹ in [26]. The explicit solution of the one and two magnon problem allowed us to understand that the deviation from the “ideal string” configuration vanishes exponentially with the chain length. In other terms, the string solutions are asymptotic.

In this chapter we consider the case of solutions with an arbitrary number of magnons. We are able to show that, in the asymptotic regime $L \rightarrow \infty$, the scattering of magnons associated to the bound states discussed above is described by the BDS ansatz.

The finite size corrections may be evaluated, similarly to the one-magnon case, to be of the order $e^{-2\beta L}$ where β is the typical strength of the binding $\sinh \beta \sim 1/g$. At weak coupling, or in the perturbative regime, these corrections are of order g^{2L} , as expected.

For reasons of simplicity, we are concentrating first on magnons with real momentum, that is strings containing only one u . In this situation, the momenta q_n appear in complex conjugate pairs. Let us choose the labels such that the first M momenta have a positive imaginary part β_n , while the last M momenta have a negative imaginary part. With the experience gained from the one- and two-magnon case we denote

$$\begin{aligned} q_n - \phi &= s_n \frac{\pi}{2} + \frac{p_n}{2} + i\beta_n, \\ q_{n+M} - \phi &= s_n \frac{\pi}{2} + \frac{p_n}{2} - i\beta_n, \quad \beta_n > 0, \quad n = 1, \dots, M. \end{aligned} \quad (59)$$

where p_n will be the magnon momentum, and $s_n = \text{sign } p_n$ ¹⁰. If L is large, the left hand side of (37) vanishes exponentially for $n = 1, \dots, M$ and diverges for $n = M+1, \dots, 2M$. Therefore, for L infinite and for any $n = 1, \dots, M$ there exist one u , which will be called u_n , such that

$$u_n - i/2 = \sqrt{2}g \sin(q_n - \phi), \quad u_n + i/2 = \sqrt{2}g \sin(q_{n+M} - \phi), \quad (60)$$

or, equivalently,

$$u_n \pm i/2 = \sqrt{2}g s_n \cos\left(\frac{p_n}{2} \mp i\beta_n\right). \quad (61)$$

In particular, equation (61) allows to determine the inverse size of the bound state, β_n , in terms of the magnon momentum p_n

$$\sinh \beta_n = \frac{1}{2\sqrt{2}g s_n \sin \frac{p_n}{2}} = \frac{1}{2\sqrt{2}g |\sin \frac{p_n}{2}|}. \quad (62)$$

⁸In our notation, they should be called q - u strings.

⁹In the repulsive case considered by Takahashi, the energy of such a bound state is greater than the energy of its constituents, but the wave function is localized in space, so they can still be called bound states.

¹⁰We assume that $p_n \in (-\pi, \pi)$, meaning that the real part of $q_n - \phi$ ranges from $\pi/2$ to $3\pi/2$. It is interesting to note that there is no consistent solution with $q_n - \phi \in (-\pi/2, \pi/2)$. Such a solution would imply a negative energy for the corresponding magnon, which is unphysical.

and to find the relation between u_n and p_n

$$u_n = \sqrt{2}g s_n \cos \frac{p_n}{2} \cosh \beta_n = \frac{1}{2} \cot \frac{p_n}{2} \sqrt{1 + 8g^2 \sin^2 \frac{p_n}{2}}, \quad (63)$$

which is nothing else than the relation (2) of the BDS Bethe ansatz. The next step is to eliminate the fermion momenta q_n from the dual Lieb-Wu equations and replace them by the magnon rapidities u_n . In order to perform this task, we multiply the equations number n and $n + M$ in (37), so that the real parts in the exponential mutually cancel

$$e^{i(p_n + 2\phi + s_n \pi)L} = - \prod_{\substack{j=1 \\ j \neq n}}^M \frac{u_n - u_j + i}{u_n - u_j - i}. \quad (64)$$

Under the condition $e^{2i\phi L} = (-1)^{L+1}$, which is satisfied due to our choice of the twist (15), equation (64) is identical to the BDS Bethe ansatz equation (1). The second dual Lieb-Wu equation (38) is automatically satisfied, while the energy becomes

$$\begin{aligned} E &= -\frac{\sqrt{2}}{g} \sum_{n=1}^M (\cos(q_n - \phi) + \cos(q_{n+M} - \phi)) - \frac{M}{g^2} \\ &= \frac{2\sqrt{2}}{g} \sum_{n=1}^M \left| \sin \frac{p_n}{2} \right| \cosh \beta_n - \frac{M}{g^2} = \sum_{n=1}^M \frac{1}{g^2} \left(\sqrt{1 + 8g^2 \sin^2 \frac{p_n}{2}} - 1 \right). \end{aligned} \quad (65)$$

which is, again, the BDS result (3).

This proof can be easily extended to the situation when the magnon momenta p_n are not all real. This may be the case for strings containing more than a single u . We can think of such a string as being composed of several one-magnon strings, each centered to a complex momentum p_n . The above equations are still valid, under the provision that s_n is defined as the sign of the real part of p_n , $s_n = \text{sign Re } p_n$. Let us note that s_n is well defined if u_n is finite. Of course, β_n are not real any more but they are defined by the first equality in (62).

5 Four-Loop Konishi and the Wrapping Problem

The Hubbard model is capable of naturally dealing with the “wrapping problem” [7]. The latter is a fundamental difficulty for a long-range spin chain, where one has to decide how to interpret the Hamiltonian when the interaction range reaches the size of the system¹¹.

¹¹If there are only two-body long-range interactions, as e.g. in the Inozemtsev long-range spin chain [13], the problem may be circumvented by periodizing the two-body interaction potential. If there are also multi-body interactions, as occurs in the long-range spin chains appearing in perturbative gauge theory, it is just not clear how to deal with this problem in a natural fashion. See [27] for a very recent discussion of these problems.

Let us state the prediction of the Hubbard model for the anomalous dimension of the lowest non-trivial state, the Konishi field, with $L = 4$ and $M = 2$, to e.g. eight-loop order¹². It is easily obtained using e.g. the tool in Appendix B:

$$E_{\text{Hubbard}} = 6 - 12g^2 + 42g^4 - 318g^6 + 4524g^8 - 63786g^{10} + 783924g^{12} - 8728086g^{14} + \dots \quad (66)$$

The four-loop prediction, $-318g^6$, is the first order where wrapping occurs. The result should be contrasted to the BDS Bethe ansatz, which, when we “illegally” apply it beyond wrapping order, yields (again, we used the program described in Appendix B)

$$E_{\text{BDS}} = 6 - 12g^2 + 42g^4 - \frac{705}{4}g^6 + \frac{6627}{8}g^8 - \frac{67287}{16}g^{10} + \frac{359655}{16}g^{12} - \frac{7964283}{64}g^{14} + \dots \quad (67)$$

We can now see explicitly that the perturbative results for the energy differs in the two ansätze at $\mathcal{O}(g^6)$, i.e. four loop order. The exact result for Konishi is given by a rather intricate algebraic curve. Note that the two rapidities u_1, u_2 are *not* related by the symmetry $u_1 = -u_2$.

Let us likewise contrast the results for the lowest non-BPS state with an odd length, namely $L = 5, M = 2$. The Hubbard model gives

$$E_{\text{Hubbard}} = 4 - 6g^2 + 17g^4 - \frac{115}{2}g^6 + \frac{833}{4}g^8 - \frac{6147}{8}g^{10} + \frac{44561}{16}g^{12} - \frac{303667}{32}g^{14} \quad (68)$$

while the BDS ansatz yields

$$E_{\text{BDS}} = 4 - 6g^2 + 17g^4 - \frac{115}{2}g^6 + \frac{849}{4}g^8 - \frac{6627}{8}g^{10} + \frac{53857}{16}g^{12} - \frac{451507}{32}g^{14} + \dots \quad (69)$$

In line with expectation this confirms that the perturbative results for the energy differ between Hubbard and BDS at $\mathcal{O}(g^8)$, i.e. five loop order. This is precisely where wrapping first occurs for a length five ring. The exact result is again given by an intricate algebraic curve.

6 Conclusions

The main result of this paper is the identification of the long-range BDS spin chain of [7] as an asymptotic approximation to a short-range model of itinerant fermions, the Hubbard model. The latter yields a rigorous microscopic definition of the former. It furthermore provides the Hamiltonian, which was only known, in an “effective” form, to five-loop order [7]. We have explicitly derived the emergence of this effective description to three-loop order by correcting a previously performed strong-coupling expansion of the one-dimensional Hubbard model [17]. This establishes and proves that the planar three-loop dilatation operator of $\mathcal{N} = 4$ gauge theory is, in the $\mathfrak{su}(2)$ sector, generated by a twisted Hubbard model. We have also derived the asymptotic Bethe equations of the BDS chain from the Lieb-Wu equations of the Hubbard model.

¹²It is interesting that the coefficients seem to be all integer, at least to the order we checked.

Our identification allows to resolve the wrapping problem of the BDS chain in a, as far as we can currently see, unique fashion. It also gives a rigorous definition of *integrability* beyond wrapping order and therefore for a system of *finite* extent. Recall that the notion of “perturbative” integrability implemented in [7] requires, strictly speaking, an infinite system. This renders the BDS ansatz (1),(2),(3) only asymptotically and thus approximately valid. The, admittedly more complicated, Lieb-Wu equations (30),(31),(32) or (37),(38),(39) are the generalization of the BDS equations to strictly finite systems and to arbitrary values of the coupling constant g . Their firm base is an underlying S-matrix satisfying the Yang-Baxter equation [15]. What is more, the Hubbard model may be included into the rigorous framework of the quantum inverse scattering method. In fact, Shastry discovered its R-matrix [29], and Ramos and Martins [30] diagonalized the model by algebraic Bethe ansatz. These results therefore also embed the BDS spin chain into the systematic inverse scattering formalism.

We have not been able to find the “effective” ansatz (1),(2),(3), which significantly simplifies the nested Lieb-Wu equations at half-filling up to wrapping terms, in the (vast) literature on the Hubbard model [16]. This striking simplification seems to be a discrete and generic generalization of the decoupling phenomenon of the system of thermodynamic integral equations for the antiferromagnetic ground state energy, as originally observed by Lieb and Wu [15].

Our results strongly indicate that, sadly, wrapping interactions are *not* able to explain the three-loop discrepancies [22, 6] between gauge and string theory, as was originally hoped for in a proposal in [7]. As discussed in chapter 4, the Hubbard model simply does not seem to allow for two distinct ways to form the small BMN parameter $\lambda' \sim g^2/L^2$. Put differently, in the Hubbard model there is no order of limits problem, and wrappings just lead to $\mathcal{O}(g^{2L})$ effects which disappear in the BMN limit. This negative result seems to be in agreement with the complementary findings in [21].

Actually, we cannot currently exclude that there might be other, similar (modified, generalized Hubbard?) models which also agree with BDS up to wrapping order, but differ from our current proposal in the wrapping terms. However, even if these exist, we find it hard to believe that they will allow for a new way to form the BMN parameter λ' at strong coupling.

These questions should be distinguished from the related, but distinct (since the AdS/CFT discrepancy appears at three loops) issue whether the BDS-Hubbard system is actually describing the gauge theory’s $\mathfrak{su}(2)$ dilatation operator *at and beyond* four-loop order. It is of course logically possible that the latter is *not* asymptotically given by the BDS chain at some loop order larger than three. Assuming integrability, we would then conclude that BMN scaling should break down at, or beyond, four-loop order, cf. [7]. Then the BMN proposal [8] along with the arguments of [31] would be invalid for the gauge side.

It should be clear from the preceding discussion that *we are in dire need of a perturbative four-loop anomalous dimension computation in $\mathcal{N} = 4$ gauge field theory*. Of particular importance would be the four-loop dimension of the Konishi field. If it turns out to agree with our finding in this paper ($-318g^8$), our attempts to identify the $\mathfrak{su}(2)$ sector of the $\mathcal{N} = 4$ dilatation operator with the Hubbard Hamiltonian will, in our opinion, become very plausible. If it disagrees, the search for the correct all-loop dilatation

operator will have to be continued.

Strong additional constraints come from considering the integrable structure of the dilatation operator beyond the $\mathfrak{su}(2)$ sector. The $\mathfrak{su}(2)$ three-loop dilatation operator [3] is naturally embedded in the maximally compact closed sector $\mathfrak{su}(2|3)$ [4]. The asymptotic BDS ansatz may also be lifted in a very natural fashion to this larger sector [32, 33]. Here “natural” means that the ansatz (1) contains BDS as a limit, (2) diagonalizes the three-loop dilatation operator in the $\mathfrak{su}(2|3)$ sector, which is firmly established [4, 5], and (3) may be derived from a factorized S-matrix satisfying the Yang-Baxter algebra [32, 33, 34]. Actually, the asymptotic BDS ansatz may even be modified to include non-compact sectors such as $\mathfrak{sl}(2)$ [32], and lifted to the *complete* theory [33], with symmetry $\mathfrak{psu}(2, 2|4)$. Again, the construction seems compelling as it may be shown that (1) the Bethe ansatz correctly diagonalizes to three loops twist-two operators [32] whose dimensions are known from the work of [36, 37], (2) it also diagonalizes a twist-three operator to two loops which was confirmed using field theory in [38]. In fact, it may be proved (3) that it diagonalizes to two loops the dilatation operator in the $\mathfrak{psu}(1, 1|2)$ sector which has recently been computed by Zwiebel, using algebraic means in [39], and (4) for $\mathfrak{sl}(2)$ one may derive the ansatz at two loops directly from the field theory [40]. Finally, the entire $\mathfrak{psu}(2, 2|4)$ ansatz may again be derived from an S-matrix satisfying the Yang-Baxter equation [34]. It is important to note that the structure of the S-matrix, as well as, as a consequence, the nested asymptotic Bethe ansatz, are nearly completely constrained by symmetry [34], up to a global scattering “dressing factor” [25, 32, 33]. This means that e.g. the Inozemtsev model [6] is ruled out [34] as an all-loop candidate. It also means that a possible breakdown of BMN scaling, confer the discussion above, could only be caused by the dressing factor, starting at or above four loops. See also [27]. Incidentally, it would be very interesting to understand whether short-range formulations also exist for other (or even all) asymptotically integrable long-range spin chains [35],[27].

From the preceding discussion we conclude that it will be crucial to investigate whether the twisted Hubbard model may be extended to sectors other than $\mathfrak{su}(2)$, and eventually to the full symmetry algebra $\mathfrak{psu}(2, 2|4)$. A further constraint will be that this extension asymptotically yields the Bethe equations of [33]. It would be exciting if finding the proper short-range formulation of the full dilatation operator resulted, when restricting to $\mathfrak{su}(2)$, in a model that also asymptotically generates BDS but differed from the specific Hubbard Hamiltonian we discussed in this paper. At any rate we find it likely, given the results of this work, that such a *short-range* formulation of the gauge theory dilatation operator exists. It will be interesting to see whether the latter also eliminates the length-changing operations which appear in the current long-range formulation as a “dynamic” spin chain [4].

An intriguing if puzzling aspect of our formulation is that the Hubbard model has many more states than the perturbative gauge theory in the $\mathfrak{su}(2)$ sector. For a length L operator we have roughly $2^L/L$ cyclic states in the spin chain and in the gauge theory, and $4^L/L$ cyclic states in the Hubbard model, cf. section 4.1. Is this an artifact of the incompleteness, or erroneousness, of our identification, or a first hint at a rich non-perturbative structure of planar $\mathcal{N} = 4$ gauge theory? Does it possibly tell us that the fields appearing in the Lagrangian of the $\mathcal{N} = 4$ theory are composites of more fundamental degrees of freedom (such as the “electrons” of our model)? Note also that

the Hubbard model has a second “hidden” $\mathfrak{su}(2)$ symmetry [16]. Our twisting procedure actually breaks the symmetry through the boundary conditions. Thermodynamically, however, i.e. in the large L limit, the symmetry is still present. The mechanism is reminiscent of the considerations of Minahan [23], but the details appear to be different.

Concerning the proposed AdS/CFT duality [41], our result, for the moment, just deepens the mystery of the vexing “three-loop discrepancies” of [22],[6]. The dual string theory is classically integrable [42], which leads to a complete solution of classical string motions [43] in terms of an algebraic curve [44]. The uncovered integrable structure is very similar [45] but different [6],[7] from the one of the (thermodynamic limit of) gauge theory. Much evidence was found that the string theory is also *quantum* integrable. This can be established by a spectroscopic analysis of the spectrum of strings in the near-BMN limit [22],[46], which shows that it may be “phenomenologically” explained by factorized scattering [25],[32]. Again, the integrable structure is similar but, at the moment, appears to differ. Some progress has also been made towards deriving quantum integrability directly from the string sigma model [47].

It would be exciting to find a Hubbard-type short-range model which reproduces the string theory results. Recently it was demonstrated by Mann and Polchinski [48] that conformal quantum sigma models can give Bethe equations whose classical limit reproduces (in the $\mathfrak{su}(2)$ sector) the bootstrap equations of [44]. There is one structural feature of their approach which strongly resembles the considerations in this paper: In order to be able to treat the $\mathfrak{su}(2)$ case they need to employ a *nested* Bethe ansatz, which is reminiscent of the Lieb-Wu equations of the Hubbard model. A difference, however, is that in their case elementary excitations of the same type are interacting with a non-trivial S-matrix, while in our model identical fermions are free.

Acknowledgments

D.S. and M.S. thank the *Kavli Institute for Theoretical Physics*, Santa Barbara, for hospitality. D.S. thanks the *Albert-Einstein-Institut*, Potsdam, for hospitality. We also thank Niklas Beisert, David Berenstein, Zvi Bern, Burkhard Eden, Sergey Frolov, Frank Göhmann, David Gross, Volodya Kazakov, Ivan Kostov, Juan Maldacena, Nelia Mann, Jan Plefka, Joe Polchinski, Radu Roiban and Aureliano Skirzewski for their interest and for helpful discussions. This research was supported in part by the National Science Foundation under Grant No. PHY99-07949.

A Effective Spin Hamiltonian: Perturbation Theory and Computation Schemes

A.1 Perturbation Theory for Degenerate Systems

Consider a system which is described by a Hamiltonian H_0 . Assume that the spectrum of H_0 is discrete, and that the system is in a stable state with energy E_a^0 . In general the subspace U_a corresponding to an eigenvalue E_a^0 has dimension g_a , where g_a is the degeneracy of the level E_a^0 . Let us denote by $|u_1\rangle, \dots, |u_{g_a}\rangle$ the vectors spanning U_a . What happens if we add a small interaction $+\lambda V$? In general we have a set of subspaces

$\mathcal{E}_1, \dots, \mathcal{E}_n$, for which $\mathcal{E}_1(\lambda) + \dots + \mathcal{E}_n(\lambda) \rightarrow U_a$ when $\lambda \rightarrow 0$ and $\dim(\mathcal{E}_1 + \dots + \mathcal{E}_n) = g_a$. If λ is sufficiently small, we may assume that there exists a one-to-one correspondence between U_a and $W = \mathcal{E}_1(\lambda) + \dots + \mathcal{E}_n(\lambda)$. This correspondence is established by a transformation, to be found. Let $|\phi\rangle$ be any state in the Hilbert space generated by H_0 . Its projection on U_a is formally realized by :

$$P_0 = \frac{1}{2\pi i} \oint_{C_0} \frac{dz}{z - H_0}, \quad (70)$$

where the contour C_0 is enclosing only the eigenvalue E_a^0 of H_0 . From this discussion we conclude that the projector on the subspace W is given by

$$P = \frac{1}{2\pi i} \oint_C \frac{dz}{z - H_0 - \lambda V}. \quad (71)$$

The contour C encloses the $n + 1$ points $E_a^0, E_1(\lambda), \dots, E_n(\lambda)$ (the last n collapse to E_a^0 when $\lambda \rightarrow 0$). Using the identity

$$\begin{aligned} \frac{1}{z - H_0 - \lambda V} &= \frac{1}{z - H_0} (z - H_0 + \lambda V - \lambda V) \frac{1}{z - H_0 - \lambda V} = \frac{1}{z - H_0} \\ &+ \frac{1}{z - H_0} \lambda V \frac{1}{z - H_0 - \lambda V}, \end{aligned} \quad (72)$$

we immediately get the expansion

$$P = \frac{1}{2\pi i} \oint_C dz \frac{1}{z - H_0} \sum_{n=0}^{\infty} \lambda^n (V \frac{1}{z - H_0})^n. \quad (73)$$

Careful use of the generalized Cauchy integral formula leads to the expansion

$$P = P_0 - \sum_{n=1}^{\infty} \lambda^n \sum_{k_1 + \dots + k_{n+1} = n, k_i \geq 0} S^{k_1} V S^{k_2} V \dots V S^{k_{n+1}}, \quad (74)$$

where one defines

$$S^0 \equiv -P_0, \quad S^k = \left((1 - P_0) \frac{1}{E_0 - H_0} \right)^k \quad \text{for } k > 0. \quad (75)$$

Naively one would expect that the correspondence between U_a and W is realized by the projector P , i.e. that any state $|\psi\rangle \in W$ can be written as

$$|\psi\rangle = P|\phi\rangle, \quad (76)$$

where $|\phi\rangle$ is some vector in U_a . This would allow us to bring the eigenvalue problem

$$H|\psi\rangle = E|\psi\rangle, \quad (77)$$

with

$$H = H_0 + \lambda V, \quad (78)$$

to the subspace U_a

$$HP|\phi\rangle = EP|\phi\rangle. \quad (79)$$

The disadvantage of this procedure is a nontrivial overlap EP on the r.h.s. of (79), i.e. EP is not proportional to the identity map. Furthermore P does not preserve the norm of the states. The problem of this effective overlap has been solved by Löwdin [20]. One introduces renormalized states (which are still states from U_a)

$$|\hat{\phi}\rangle = (P_0PP_0)^{1/2}|\phi\rangle, \quad (80)$$

and thus one is lead to the introduction of the $U_a \leftrightarrow W$ correspondence operator Γ :

$$\Gamma = PP_0(P_0PP_0)^{-1/2}, \quad (81)$$

where

$$(P_0PP_0)^{-1/2} \equiv P_0 + \sum_{n=1}^{\infty} \frac{1}{4^n} \binom{2n}{n} \left[P_0(P_0 - P)P_0 \right]^n, \quad (82)$$

plus an analogous formula for $(P_0PP_0)^{1/2}$. One can then prove that $\Gamma^\dagger\Gamma = P_0$, so

$$(\Gamma|\phi\rangle, \Gamma|\phi'\rangle) = (|\phi\rangle, |\phi'\rangle), \quad (83)$$

and the transformation preserves the norm. We may now substitute equation (77) by an effective equation

$$(h - E)|\phi'\rangle = 0, \quad (84)$$

where

$$h \equiv \Gamma^\dagger H \Gamma. \quad (85)$$

The operator h is the *effective* Hamiltonian. To find it for the Hubbard model at half-filling we put

$$H_0 = tU \sum_{i=1}^L c_{i\uparrow}^\dagger c_{i\uparrow} c_{i\downarrow}^\dagger c_{i\downarrow}, \quad V = \sum_{i<j}^L t_{ij} (X_{ij} + X_{ji}), \quad X_{ij} = \sum_{\sigma=\uparrow,\downarrow} c_{i\sigma}^\dagger c_{j\sigma}, \quad (86)$$

with U_a being the ground-state subspace \mathcal{E}_0 we defined at the beginning of this section. One may show that the odd powers disappear from the expansion of h , as one would expect from the 'hopping and hopping back' random walk interpretation:

$$h = \lambda^2 h_2 + \lambda^4 h_4 + \lambda^6 h_6 + \dots. \quad (87)$$

A.2 Computation Schemes

Performing the computations can be divided into three stages:

Stage 1 This stage consists of evaluating the effective Hamiltonian (85) to a given order. This is a tedious problem beyond the first few orders. One can however use that $E_a^0 = 0$ for the half-filled Hubbard model, whence in order to get h to n -th order, one only needs to evaluate Γ to $(n - 1)$ -th order. Furthermore it can be proved that any term of the form

$$P_0 V S^{k_1} V S^{k_2} \dots V S^{k_{n-1}} V P_0, \quad k_i \geq 1, \quad (88)$$

for odd n vanishes identically. This two observations greatly speed up the calculations. A program in FORM (see [49]) was written to perform this stage of the calculations. The result we found up to three-loop reads

$$\begin{aligned} h = & +\lambda^2(P_0 V S V P_0) + \lambda^4(P_0 V S V S V S V P_0 - \frac{1}{2}P_0 V S V P_0 V S S V P_0 \\ & - \frac{1}{2}P_0 V S S V P_0 V S V P_0) \\ & + \lambda^6(P_0 V S V S V S V S V S V P_0 - \frac{1}{2}P_0 V S V S V S V P_0 V S S V P_0 \\ & - \frac{1}{2}P_0 V S V S V S S V P_0 V S V P_0 - \frac{1}{2}P_0 V S V S S V S V P_0 V S V P_0 \\ & - \frac{1}{2}P_0 V S V P_0 V S V S V S S V P_0 - \frac{1}{2}P_0 V S V P_0 V S V S S V S V P_0 \\ & + \frac{1}{2}P_0 V S V P_0 V S V P_0 V S S S V P_0 - \frac{1}{2}P_0 V S V P_0 V S S V S V S V P_0 \\ & + \frac{3}{8}P_0 V S V P_0 V S S V P_0 V S S V P_0 - \frac{1}{2}P_0 V S S V S V S V P_0 V S V P_0 \\ & - \frac{1}{2}P_0 V S S V P_0 V S V S V S V P_0 + \frac{1}{4}P_0 V S S V P_0 V S V P_0 V S S V P_0 \\ & + \frac{3}{8}P_0 V S S V P_0 V S S V P_0 V S V P_0 + \frac{1}{2}P_0 V S S S V P_0 V S V P_0 V S V P_0), \end{aligned} \quad (89)$$

It is indeed equivalent to the expansion obtained by Klein and Seitz in [17].

Stage 2 This stage consists of substituting (86) into h_{2n} as calculated in stage 1. The process of substitution can be well visualized by assigning to each X_{ij} an oriented line, starting at j and ending in i , see Fig.1a. Products of the X operators are represented by an oriented set of arrows, with the understanding that the lowest lying arrow corresponds to the last operator in the product. A curly bracket around a set of arrows denotes a sum over different locations of the arrows. One can interpret these diagrams as virtual displacements of spins. It was proved that the perturbation expansion consists only of *linked* diagrams (see [17] for details). The rather technical reason for this are the $(P_0 P P_0)^{-1/2}$ terms in (85), cf. the discussion in the paper by Klein and Seitz [17]. Each diagram is multiplied by a suitable factor following from the structure of the h_{2n} expansion.

Stage 3 This final stage consists of evaluating the diagrams obtained in stage 2. Since the diagrams are closed, for each lattice site i the number of arrows starting and ending at i is the same. Keeping in mind the definition of X_{ij} , and using anti-commutation relations for every diagram connecting r lattice sites, we can assign each diagram linear combinations of terms of the form

$$N(i_1, \tau_1, \tau_2) \dots N(i_k, \tau_{2k-1}, \tau_{2k}) \quad k \leq r, \quad (90)$$

where

$$N(i, \tau, \sigma) = c_{i\tau}^\dagger c_{i\sigma}. \quad (91)$$

Furthermore one may rewrite each diagram in terms of spin components by means of the relations

$$S_i^+ = c_{i\uparrow}^\dagger c_{i\downarrow}, \quad S_i^- = c_{i\downarrow}^\dagger c_{i\uparrow}, \quad (92)$$

and

$$S_i^z = \frac{1}{2}(c_{i\uparrow}^\dagger c_{i\uparrow} - c_{i\downarrow}^\dagger c_{i\downarrow}) \simeq c_{i\uparrow}^\dagger c_{i\uparrow} - \frac{1}{2} \simeq 1/2 - c_{i\downarrow}^\dagger c_{i\downarrow}, \quad (93)$$

where the last two equalities are only valid when acting on states with a single electron per site. This is however our case, after putting the diagrams into the form (90). The whole procedure is carried out in FORM.

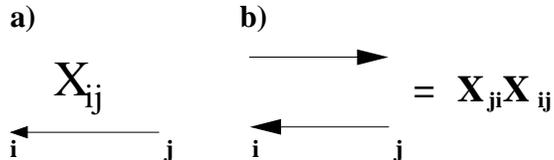


FIG. 1. a) To each X_{ij} operator we assign an oriented arrow emerging from site j. b) A product of operators is represented by an ordered set of arrows. The lowest lying arrow corresponds to the last operator in the product.

A.3 Twist factors

Equation (14) differs from (23) by the fact, that each hopping to the right is multiplied by a factor of $e^{i\phi}$, while hopping to the left gets an extra factor of $e^{-i\phi}$. Since the perturbation theory consists only of closed diagrams, we conclude that these factors cancel at the end.

This reasoning is generally true for long spin chains. A notable exception is when the chain is sufficiently short such that a spin can hop around the ring. This happens for example at two loops and $L = 4$. There are two diagrams corresponding to this process. They are related to each other by reversing all arrows in one of them. The two diagrams have thus weights differing by factors of opposite signature ($e^{i\phi L} = i$ and $e^{-i\phi L} = -i$, c.f. (15)) and they therefore cancel each other. Thus putting the twist results in eliminating these unwanted demi-wrapping terms.

B Mathematica Code for the Perturbative Solution of the Lieb-Wu Equations

In this appendix we will collect some `Mathematica` routines which allow for the immediate solution of the BDS equations (1),(2),(3) and the Lieb-Wu equations (30),(31),(32) for systems of relatively small lengths L once the one-loop solution is known. The necessary input is thus the collection of one-loop Bethe roots $\{u_k\}$, i.e. the solution of (34) for the state in question. The one-loop roots for the first few states may be found in appendix A of [7]. The below routines may therefore be used to check our claims about the agreement (below wrapping order) and disagreement (at and beyond wrapping order) between the

BDS ansatz and the Lieb-Wu ansatz on various specific states. There is however one restriction where the program does not directly apply: There are a number of “singular” states [11, 7] with three special unpaired one-loop roots $u_1 = -\frac{i}{2}, u_2 = 0, u_3 = \frac{i}{2}$ which require regularization.

These definitions set up the algorithm:

```

uu[k_, l_] := Sum[u[k, s]g^s, {s, 0, 2l - 2}];

qq[n_, l_] := Sum[q[n, s]g^s, {s, 0, 2l - 2}];

\[\Phi][L_] := If[EvenQ[L] == True, Pi/(2L), 0];

x[u_] := u/2(1 + Sqrt[1 - 2 g^2/u^2])

BDS[L_, M_, l_] :=
Table[(x[uu[k, l] + I/2]/x[uu[k, l] - I/2])^L +
Product[(uu[k, l] - uu[j, l] + I)/(uu[k, l] - uu[j, l] - I),
{j, 1, M}], {k, 1, M}]

EBDS[M_, l_] := Sum[I/x[uu[k, l] + I/2] - I/x[uu[k, l] - I/2], {k, M}]

LW1[L_, M_, l_] :=Table[Exp[I qq[n, l] L] -Product[
(uu[j, l] - Sqrt[2]g Sin[(qq[n, l] + \[\Phi][L]) - I/2]/
(uu[j, l] - Sqrt[2]g Sin[(qq[n, l] + \[\Phi][L]) + I/2]),{j, M}], {n, L}]

LW2[L_, M_, l_] := Table[Product[
(uu[k, l] - Sqrt[2]g Sin[qq[n, l] + \[\Phi][L] + I/2]/
(uu[k, l] - Sqrt[2]g Sin[qq[n, l] + \[\Phi][L] - I/2]),{n, L}] +
Product[(uu[k, l] - uu[j, l] + I)/(uu[k, l] - uu[j, l] - I),
{j, 1, M}], {k, 1, M}]

ELW[L_, l_] := Sqrt[2]/g Sum[Cos[(qq[n, l] + \[\Phi][L])], {n, L}]

```

In order to find the prediction of the BDS chain for e.g. the state with $L = 5$ and $M = 2$, where the two one-loop Bethe roots are $u_1 = \frac{1}{2}$ and $u_2 = -\frac{1}{2}$, we then compute, to e.g. $l = 8$ loops,

```

Clear[u]; Clear[q]; L = 5; M = 2; l = 8;

u[1, 0] = 0.5; u[2, 0] = -0.5;

Do[xxx = Chop[Series[BDS[L, M, 2l + 1], {g, 0, 1l - 2}]];
yyy = Flatten[Chop[Solve[Coefficient[xxx, g, 1l - 2] == 0]]];
Do[u[k, 1l - 2] = yyy[[k]][[2]], {k, 1, M}], {1l, 3, 2l + 1}];
Series[EBDS[M, 2l], {g, 0, 2l - 2}] // Chop // Rationalize

```

If we are, on the other hand interested in the correct result of the Hubbard model, we compute instead

```
Clear[u]; Clear[q]; L = 5; M = 2; l = 8;

u[1, 0] = 0.5; u[2, 0] = -0.5;

Do[q[n, 0] = 2 Pi/L(n - 1), {n, 1, L}];
Do[xxx = Chop[Series[LW2[L, M, 2l + 1], {g, 0, ll - 2}]];
yyy = Flatten[Chop[Solve[Coefficient[xxx, g, ll - 2] == 0]]];
Do[u[k, ll - 2] = yyy[[k]][[2]], {k, 1, M}];
uuu = Chop[Series[LW1[L, M, 2l + 1], {g, 0, ll - 2}]];
vvv = Flatten[Chop[Solve[Coefficient[uuu, g, ll - 2] == 0]]];
Do[q[n, ll - 2] = vvv[[n]][[2]], {n, 1, L}], {ll, 3, 2 l + 1}];
Series[ELW[L, 2l + 1], {g, 0, 2l - 2}] // Chop // Rationalize
```

C Generic Twists

In this appendix we study all the possible twisted boundary conditions for the Hubbard model which are compatible with integrability and the way they affect the Lieb-Wu equations. The results are essentially due to Yue and Deguchi [28], who studied the twisted boundary conditions associated to a model of two coupled XY models which, upon a Jordan-Wigner transformation, is equivalent to the twisted Hubbard model. Translating their results in terms of the Hubbard model, we obtain that the twists depend on six different constants

$$\phi_{\uparrow} = a_{\uparrow} + N b_{\uparrow} + M c_{\uparrow} \quad (94)$$

$$\phi_{\downarrow} = a_{\downarrow} + N b_{\downarrow} + M c_{\downarrow} \quad (95)$$

while the corresponding version of the Lieb-Wu equations is

$$e^{i\tilde{q}_n L} = \prod_{j=1}^M \frac{u_j - \sqrt{2}g \sin(\tilde{q}_n + \phi_{\uparrow}) - i/2}{u_j - \sqrt{2}g \sin(\tilde{q}_n + \phi_{\uparrow}) + i/2}, \quad n = 1, \dots, N \quad (96)$$

$$\prod_{n=1}^N \frac{u_k - \sqrt{2}g \sin(\tilde{q}_n + \phi_{\uparrow}) + i/2}{u_k - \sqrt{2}g \sin(\tilde{q}_n + \phi_{\uparrow}) - i/2} = e^{iL(\phi_{\downarrow} - \phi_{\uparrow})} \prod_{\substack{j=1 \\ j \neq k}}^M \frac{u_k - u_j + i}{u_k - u_j - i}. \quad k = 1, \dots, M$$

The energy of the corresponding states is given by

$$E = \frac{\sqrt{2}}{g} \sum_{n=1}^N \cos(\tilde{q}_n + \phi_{\uparrow}). \quad (97)$$

After the duality transformation, the fermion number becomes $L - N + 2M$, g changes sign and $\phi_\uparrow \rightarrow \pi - \phi_\uparrow$, and $\phi_\downarrow \rightarrow \phi_\downarrow$. The dual Lieb-Wu equations are, for generic twist

$$e^{iq_n L} = \prod_{j=1}^M \frac{u_j - \sqrt{2}g \sin(q_n - \phi_\uparrow) - i/2}{u_j - \sqrt{2}g \sin(q_n - \phi_\uparrow) + i/2}, \quad n = 1, \dots, L - N + 2M \quad (98)$$

$$\prod_{n=1}^{L-N+2M} \frac{u_k - \sqrt{2}g \sin(q_n - \phi_\uparrow) + i/2}{u_k - \sqrt{2}g \sin(q_n - \phi_\uparrow) - i/2} = e^{iL(\phi_\downarrow + \phi_\uparrow - \pi)} \prod_{\substack{j=1 \\ j \neq k}}^M \frac{u_k - u_j + i}{u_k - u_j - i}. \quad k = 1, \dots, M$$

while the energy is

$$E = -\frac{M}{g^2} - \frac{\sqrt{2}}{g} \sum_{n=1}^{L-N+2M} \cos(q_n - \phi_\uparrow). \quad (99)$$

To obtain the BDS ansatz, the following conditions on the twists have to be satisfied

$$e^{iL(2\phi_\uparrow - \pi)} = e^{iL(\phi_\downarrow + \phi_\uparrow - \pi)} = -1, \quad \text{or} \quad \phi_\uparrow = \phi_\downarrow = \frac{\pi(L+1)}{2L} \bmod \frac{\pi}{L}. \quad (100)$$

These are exactly the values we used in (15), so we infer that there is no other possibility to choose the twists compatible with the BDS ansatz.

D Further Details on the One-Magnon Problem

In section 4.1 we discussed how to account for all states of the twisted Hamiltonian acting on $L - 1$ up spins and $M = 1$ down spin. Recall that in the Hubbard model this corresponds to a *two-body* problem, hence there are L^2 states. L of these states are bound states, whose dispersion law (48) coincides with the one of the magnons in the BDS chain. This law turns, using $p = 2\pi n/L$, into the BMN square-root formula

$$g^2 E \simeq -1 + \sqrt{1 + \lambda' n^2} \quad (101)$$

if we scale $\lambda = 8\pi^2 g^2 \rightarrow \infty$, $L \rightarrow \infty$ while holding $\lambda' = \lambda/L^2$ fixed. As we showed in sections 4.2 and 4.3, the scattering of these bound states is as in the near-BMN limit of the BDS chain. It is therefore, at third order $(\lambda')^3$, incompatible with the predictions of string theory [22].

One potential way out of this trouble would be to find other states in our model which scatter as in string theory. A prerequisite is that the coupling constant dependence of the dispersion law of such candidate states is again as in (101), with, possibly, a different constant part. In particular, among the real solutions we identified in section 4.1, there were states of exact dimension $\Delta = L - 1$ which resembled ‘‘BPS states’’. Let us therefore work out the dispersion law of the nearby ‘‘near-BPS’’ states. This requires studying the solutions of (55) for small $q = \pi/L n$ and large g . Expressing (55) through the BMN coupling λ' , we find

$$\sin(b) = \frac{1}{\sqrt{\lambda' n}} \tan(bL). \quad (102)$$

Since this equation should hold as $\lambda' \rightarrow 0$, we recover the $L - 1$ mode numbers m (54):

$$b = \frac{\pi}{L} m + \frac{\delta b_m}{L}. \quad (103)$$

Now, δb_m should be at most of order $\mathcal{O}(1)$, i.e. it should not be too large so as to move out of the branch of $\tan(b_m L)$ defined by (103), and should tend to zero if $\sqrt{\lambda'} n \rightarrow 0$. This yields from (102) $\delta b_m \simeq \sqrt{\lambda'} n \sin(\frac{\pi}{L} m)$. Substitution into the expression for the energy of the real solutions

$$E = -\frac{1}{g^2} + \frac{2\sqrt{2}}{g} \sin(q) \cos(b) \quad (104)$$

gives for the dimension Δ

$$\Delta = L - 1 + \sqrt{\lambda'} n \cos\left(\frac{\pi}{L} m\right) - \frac{1}{L} \lambda' n^2 \sin^2\left(\frac{\pi}{L} m\right) + \mathcal{O}(1/L). \quad (105)$$

We see that we generically lift the $L - 1$ degenerate ‘‘BPS-states’’ with a term non-analytic in λ' . If we concentrate on mode numbers close to $m \simeq L/2$ we can suppress the non-analytic $\sqrt{\lambda'}$ term. The next term is then analytic in λ' , but *subleading* in $1/L$. It is interesting to note that there is a possibility to reproduce a BMN-like dispersion relation, by choosing m such that

$$\cos\left(\frac{\pi}{L} m\right) = \frac{1}{2} \sqrt{\lambda'} n + \mathcal{O}(1/L), \quad (106)$$

so that the conformal dimension would be analytic in λ' up to terms of order $1/L$

$$\Delta = L - 1 + \frac{1}{2} \lambda' n^2 + \mathcal{O}(1/L). \quad (107)$$

However, such a choice for m is not continuous in λ' and cannot be sensibly interpreted in terms of BMN states. The ‘‘BPS-states’’ we found are thus very different from the usual ones, and the BMN states may not be expected to hide among the continuum of real solutions.

Finally note that any one of the L bound states of section 4.1 can disappear¹³ if g is very close to L . One may show that in this case a further real solution with mode number $m = 0$, which generically does not correspond to a solution of (55), appears. Unfortunately this deconfinement phenomenon is also not suitable for finding the BMN states of string theory [8], as we are then not allowed to make the parameter λ' in (102) arbitrarily small.

E Alternative Proof of the BDS Equations

In this appendix we give an alternative proof to the BDS ansatz, using the original Lieb-Wu equation, with a macroscopic number of fermionic excitations. As in the original

¹³This is the so-called ‘‘redistribution phenomenon’’ [24] and is responsible for rendering all the fermion momenta real in the extreme g limit, $g \gg L$, which corresponds to the free fermion limit.

paper [15], we suppose that the fermion momenta are all real and they form, in the continuous limit, a continuous density. This proof is less effective than the one which starts from the dual Bethe ansatz, in the sense that the finite size corrections are not under control, and the effect of the boundary conditions (twist) is lost. However, it is interesting to see that the BDS equations are already contained in the integral equations of Lieb and Wu [15].

At half-filling, the Lieb-Wu equations can be written in the logarithmic form as

$$q_n = \phi + \frac{2\pi n}{L} - \frac{2}{L} \sum_{j=1}^M \arctan \frac{1}{2(u_j - \sqrt{2}g \sin q_n)}, \quad n = 1, \dots, L \quad (108)$$

$$2 \sum_{n=1}^L \arctan \frac{1}{2(u_k - \sqrt{2}g \sin q_n)} = 2\pi m + 2 \sum_{\substack{j=1 \\ j \neq k}}^M \arctan \frac{1}{2(u_k - u_j)}. \quad (109)$$

The choice of the branch of the logarithm in (108) is made by continuity, such that at $g = 0$ there is exactly one electron per level. For simplicity, we have removed the tilde on the variables q_n and shifted them by ϕ . Taking the derivative of the first equation with respect to q and defining the density $\rho(q) = (dn/dq)/L$ we obtain an equation for the density

$$2\pi\rho(q) = 1 + \frac{2}{L} \sum_{j=1}^M \frac{2\sqrt{2}g \cos q}{4(u_j - \sqrt{2}g \sin q)^2 + 1}. \quad (110)$$

Our purpose is to study the case of a finite (arbitrary) number of magnons, so we do not introduce a density for the magnons. Instead, we evaluate the left hand side of the second equation Lieb-Wu equation (109)

$$I(u_j) = 2L \int_{-\pi}^{\pi} dq \rho(q) \arctan \frac{1}{2(u_j - \sqrt{2}g \sin q)} \quad (111)$$

The second term in the density does not contribute to the integral $I(u)$. To compute the integral $I(u)$, we first take its derivative with respect to u , so that the cuts of the integrand disappear

$$\frac{d}{du} I(u) = \frac{L}{2\pi i} \int_{-\pi}^{\pi} dq \left(\frac{1}{u + i/2 - \sqrt{2}g \sin q} - \frac{1}{u - i/2 - \sqrt{2}g \sin q} \right). \quad (112)$$

The integral over q can be traded to a contour integral by a change of variable $z = \sqrt{2}g \sin q$

$$\frac{d}{du} I(u) = \frac{L}{2\pi i} \oint_C \frac{idz}{\sqrt{z^2 - 2g^2}} \left(\frac{1}{u^+ - z} - \frac{1}{u^- - z} \right), \quad (113)$$

where C is the contour encircling the interval $[-\sqrt{2}g, \sqrt{2}g]$ clockwise. The contour C cannot be shrunk to zero because of the obstruction created by the square root in the integrand. The integral vanishes on the contour at infinity, so we can deform the contour

C into two contours C_+ and C_- which encircle the points u^+ and u^- counterclockwise. We obtain

$$\frac{d}{du}I(u) = -iL \left(\frac{1}{\sqrt{u^+ - 2g^2}} - \frac{1}{\sqrt{u^- - 2g^2}} \right) = -iL \frac{d}{du} \ln \frac{x(u^+)}{x(u^-)}. \quad (114)$$

The constant of integration can be easily seen to be zero, since $I(\infty) = 0$. Finally, the second Lieb-Wu equation (109) takes the form

$$\left(\frac{x^+(u_k)}{x^-(u_k)} \right)^L = \prod_{\substack{j=1 \\ j \neq k}}^M \frac{u_k - u_j + i}{u_k - u_j - i}. \quad (115)$$

The magnon energy can be computed by the same means. In this case, only the second term in the density (110) contributes

$$E = \frac{\sqrt{2}}{g}L \int_{-\pi}^{\pi} dq \rho(q) \cos(q) = \frac{\sqrt{2}}{\pi g} \sum_{j=1}^M \int_{-\pi}^{\pi} dq \frac{2\sqrt{2}g \cos^2 q}{4(u_j - \sqrt{2}g \sin q)^2 + 1}. \quad (116)$$

Again, the integral can be converted into a contour integral around the same contour C which encircles the cut $[-\sqrt{2}g, \sqrt{2}g]$ clockwise

$$E = \frac{1}{g^2} \sum_{j=1}^M \oint_C \frac{dz}{2\pi i} \frac{\sqrt{z^2 - 2g^2}}{(z - u_j^+)(z - u_j^-)}. \quad (117)$$

As such, the integral does not vanish on the contour at infinity, but we can freely add to it a term which is regular across the cut and which removes the contribution from infinity

$$\begin{aligned} E &= \frac{1}{g^2} \sum_{j=1}^M \oint_C \frac{dz}{2\pi i} \frac{(\sqrt{z^2 - 2g^2} - z)}{(z - u_j^+)(z - u_j^-)} \\ &= - \sum_{j=1}^M \oint_C \frac{dz}{2\pi i} \frac{x^{-1}(z)}{(z - u_j^+)(z - u_j^-)} = i \sum_{j=1}^M \left(\frac{1}{x(u_j^+)} - \frac{1}{x(u_j^-)} \right). \end{aligned} \quad (118)$$

Of course, the reader recognizes (115) and (118) as the equations of BDS ansatz.

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