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Solving the one-dimensional Hubbard model with the Bethe Ansatz

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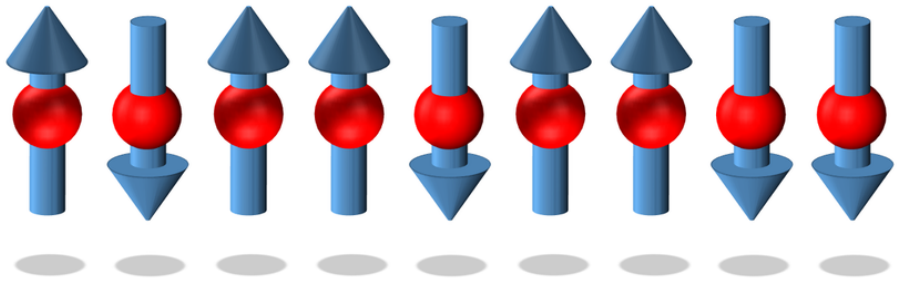

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1 Introduction to the Hubbard model and its symmetries

1.1 The Hubbard Hamiltonian

Most people at a graduate level of physics will be somewhat familiar with the one dimensional Hubbard model and it's Hamiltonian. The model arises as a simplified version of the intractable Hamiltonian of a solid, that has to take into account all interactions. The Hubbard model describes a one dimensional chain of atoms of length L with periodic boundary conditions. The electrons have same-site and nearest-neighbor interactions only. The Hamiltonian of the model is given by a sum over hopping terms and same-site terms at every site. In second quantization it is given by [1]

$$H = -t\sum_{j=1}^{L}\sum_{a=\uparrow,\downarrow}\left(c_{j,a}^{\dagger}c_{j+1,a} + c_{j+1,a}^{\dagger}c_{j,a}\right) + U\sum_{j=1}^{L} n_{j\uparrow}n_{j\downarrow}. \tag{1}$$

Here the first term corresponds to the hopping and the second accounts for the energy it costs to have two electrons with opposing spins on the same lattice site. However, for our convenience we will write the Hamiltonian as

$$H = -\sum_{j=1}^{L}\sum_{a=\uparrow,\downarrow}\left(c_{j,a}^{\dagger}c_{j+1,a} + c_{j+1,a}^{\dagger}c_{j,a}\right) + 4u\sum_{j=1}^{L} n_{j\uparrow}n_{j\downarrow}, \tag{2}$$

which corresponds to measuring in units of t. Also, we've defined $u = \frac{U}{4t}$.
The operators $c_{j,a}$ and $c_{j,a}^{\dagger}$ are the familiar annihilation and creation operators, which satisfy the canonical anticommutation relations

$$\{c_{j,a}, c_{k,b}\} = \{c_{j,a}^{\dagger}, c_{k,b}^{\dagger}\} = 0 \tag{3}$$

$$\{c_{j,a}, c_{k,b}^{\dagger}\} = \delta_{jk}\delta_{ab} \tag{4}$$

and $n_{j,a} = c_{j,a}^{\dagger}c_{j,a}$. Together with this Hamiltonian comes a set of states, known as the Wannier states, that forms a basis:

$$\mathcal{B} = \{|\boldsymbol{x}, \boldsymbol{a}\rangle \in \mathcal{H}^{(L)} | (1,\uparrow) \leq (x_1, a_1) < \cdots < (x_N, a_N) \leq (L,\downarrow)\} \tag{5}$$

where $|\boldsymbol{x}, \boldsymbol{a}\rangle = c_{x_N,a_N}^{\dagger}\ldots c_{x_1,a_1}^{\dagger}|0\rangle$ and $c_{j,a}|0\rangle = 0$ by definition and $x_j \in \{1,\ldots,L\}, a_j \in \{\uparrow,\downarrow\}$ and $j = 1,\ldots,N$, such that there are N electrons in total. These Wannier states form a basis for the total Hilbert space of the system. This space has dimension 4^L as is readily seen when considering that every site at position x_j comes with four possible states

$$|0\rangle\,,\ c_{j,\uparrow}^{\dagger}|0\rangle\,,\ c_{j,\downarrow}^{\dagger}|0\rangle\,,\ c_{j,\uparrow}^{\dagger}c_{j,\downarrow}^{\dagger}|0\rangle\,. \tag{6}$$

The Hubbard model has been quite successful in predicting some physical properties of a solid in a better way than band theory does. Examples are magnetism,

electronic properties and Mott transitions[1]. The latter will be elaborated on in a later part of this digest. But for our purposes this model is specifically interesting, because it is integrable with the Bethe Ansatz, meaning that no perturbation theory is required to extract the physical properties that we are interested in. This way of solving condensed matter systems exactly was first found by Hans Bethe in 1931 [5] and was later widely used to solve several other models, like the Lieb-Liniger model, several forms of Heisenberg chains and certain impurity models [6]. This digest will focus on the Hubbard model however, which was first solved (using the Bethe Ansatz) by Lieb and Wu in their famous 1968 article [1]. We will provide a tentative derivation for the Bethe equations and their string solutions and discuss some properties that follow from them.

1.2 Symmetries

The Hubbard Hamiltonian has some very useful symmetries. We will not discuss all of them here, but will restrict ourselves to spatial symmetries and the symmetries that deal with spin. We will start with the spatial symmetry of the system. For this, we define the permutation operator, as in [7],

$$P_{i,j} = 1 - (c_i^\dagger - c_j^\dagger)(c_i - c_j), \tag{7}$$

that permutes particles at site i and j. Also, from the canonical commutation relations it follows that

$$P_{i,j}c_i = c_j P_{i,j}. \tag{8}$$

The permutation operators form a representation of the symmetric group [8]. If we now imagine the Hubbard model with L sites and periodic boundary conditions as an L-sided polygon, we have a D_L (dihedral) symmetry group, which is a subgroup of the symmetric group, where $\frac{2\pi}{L}$ rotations and reflections that map the polygon onto itself leave the model invariant. This symmetry is known as a spatial symmetry and is generated by the shift operator and the parity operator. The shift operator is naturally defined in terms of the permutation operator as

$$\hat{U}_n = P_{n,n-1}P_{n-1,n-2}\dots P_{3,2}P_{2,1}, \tag{9}$$

such that all particles are shifted once to the left if $n = L$. Similarly $\hat{U}_L^\dagger$ shifts all particles to the right. We can generalize these operators to be spin dependent. We have for example that

$$\hat{U}_{L\uparrow} = P_{n\uparrow,n-1\uparrow}P_{n-1\uparrow,n-2\uparrow}\dots P_{3\uparrow,2\uparrow}P_{2\uparrow,1\uparrow}, \tag{10}$$

where $P_{ia,jb}$ permutes a fermion with spin a at site i with a particle with spin b at site j [9]. This operator shifts all fermions with spin up by one site to the left. We thus have

$$\hat{U} \equiv \hat{U}_L = \hat{U}_{L\uparrow}\hat{U}_{L\downarrow}. \tag{11}$$

[1] See for example [2],[3] and[4]

The parity operator is then formed from the shift operator as

$$R_L = \hat{U}_2 \dots \hat{U}_L. \tag{12}$$

The spin symmetry is twofold: we will need the symmetries that are generated by the Shiba transformation and the more familiar spin flip. We will start by defining the spin flip as

$$J^{(s)} = \prod_{j=1}^{L} P_{j\uparrow,j\downarrow}. \tag{13}$$

With the definition of $P_{ia,jb}$ given above this means that J^s indeed performs a spin flip at every site, meaning that the Z-component of the total spin changes sign. We will also need the ladder operators

$$S^+ = \sum_{j=1}^{L} c^\dagger_{j,\uparrow} c_{j,\downarrow}, \quad S^- = \sum_{j=1}^{L} c^\dagger_{j,\downarrow} c_{j,\uparrow} \tag{14}$$

and their commutation relations

$$\left[S^z, S^\pm\right] = \pm S^\pm, \ \left[S^+, S^-\right] = 2S^z. \tag{15}$$

As usual, the spin operators describe an SU(2) symmetry group of the system. The Hubbard Hamiltonian commutes with S_x, S_y and S_z and is thus invariant under this rotation.
In a similar way we can define the Shiba transformation for an even number of lattice sites as [7]

$$J^{(sh)}_a = (c^\dagger_{L,a} - c_{L,a})(c^\dagger_{L-1,a} + c_{L-1,a}) \dots (c^\dagger_{2,a} - c_{2,a})(c^\dagger_{1,a} + c_{1,a}). \tag{16}$$

These operators exchange a particle with spin a for a hole with the same spin at every site. Also notice the change of sign for every other lattice site. We can now look at the so called η-pairing symmetry, which looks similar to the spin symmetry. It is useful to define

$$J^{(sh)}_\downarrow S^+ (J^{(sh)}_\downarrow)^\dagger = \sum_{j=1}^{L} (-1)^j c^\dagger_{j,\uparrow} c^\dagger_{j,\downarrow} =: -\eta^+, \tag{17}$$

$$J^{(sh)}_\downarrow S^- (J^{(sh)}_\downarrow)^\dagger = \sum_{j=1}^{L} (-1)^j c_{j,\downarrow} c_{j,\uparrow} =: -\eta^-, \tag{18}$$

$$J^{(sh)}_\downarrow S^z (J^{(sh)}_\downarrow)^\dagger = \frac{1}{2} \sum_{j=1}^{L} (n_{j,\uparrow} + n_{j,\downarrow} - 1) = \frac{1}{2}(\hat{N} - L) =: \eta^z. \tag{19}$$

These η operators obey commutation relations as in equation (15). We can also define $\eta^x = \frac{1}{2}(\eta^+ + \eta^-)$ and $\eta^y = -\frac{i}{2}(\eta^+ - \eta^-)$. From the commutation of the

spin operators with the Hamiltonian it follows via equations (17)-(19) that the η-spin operators also commute with the Hamiltonian. Furthermore we have

$$\left[S^i, \eta^j\right] = 0, \quad i, j \in \{x, y, z\}. \tag{20}$$

The η-pairing symmetry looks like another SU(2) symmetry, but we should not forget that this symmetry only works for an even number of lattice sites. A short calculation shows that $S^z + \eta^z = \hat{N}_\uparrow - \frac{L}{2}$, which means that for even L, we will always have that either S^z and η^z are both integer or both half odd integer. The total symmetry is thus $\mathrm{SU}(2)\times\mathrm{SU}(2)/\mathbb{Z}_2 \cong \mathrm{SO}(4)$. The spin symmetry is broken by applying a magnetic field, while the η-pairing symmetry is broken by a chemical potential μ, since it does not preserve particle number.

2 Bethe Ansatz method and Lieb-Wu equations

As mentioned before, the Hubbard model can be exactly solved by the Bethe ansatz method. To solve this model means we turn the problem of solving the Schrödinger equation into the problem of finding solutions, called roots, of the so called Lieb-Wu equations. These are a set of non-linear coupled algebraic equations discovered by Lieb and Wu in their famous 1968 paper [1]. These equations contain the all the physics of the Hubbard model and determine its energy- and momentum spectrum. The problem of finding solutions of the Lieb-Wu equations is a difficult, if not impossible task (for the N-particle case). Still, they are very useful if we go to the thermodynamic limit, where only the distribution of solutions in the complex plane matters (see section 3). This is the so called string hypothesis formulated by Takahashi in 1972 [10], were we turn the problem of solving the Lieb-Wu equations into solving the Takahashi equations. In the thermodynamic limit we can express these equations as integral equations and ultimately find the roots of the initial Lieb-Wu equations. We will elaborate on the thermodynamic limit qualitatively in section 4, where the interesting properties of the system, especially in the limit that $U \to 0$, come to show.
To illustrate the effectiveness of the Bethe ansatz method we will demonstrate it on a simplified version of the Hubbard model, namely the problem with just two particles instead of the general N-particle problem. Firstly, let us detail what the N-particle problem really is. We are mostly following the derivation of [7].

2.1 The problem in first quantization

As usual in quantum mechanics, we are searching for solutions of the time-independent Schrödinger equation:

$$H\left|\psi\right\rangle = E\left|\psi\right\rangle. \tag{21}$$

We also want to solve the eigenvalue equation the shift operator defined in equation (11). This is a spatial symmetry of the system because this operator

commutes with the Hamiltonian of (2): $\left[\hat{U}, H\right] = 0$. Thus we are searching for solutions which are eigenfunctions of both these operators, i.e. we must have:

$$\hat{U}\,|\psi\rangle = \omega\,|\psi\rangle\,. \tag{22}$$

Equation (21) and (22) are in the second-quantization form, meaning that we are doing quantum field theory on the lattice and the operators are field operators. To solve the two-particle problem it is easier to switch to first quantization (just normal quantum mechanics on the lattice) for now, and express things in coordinate form. We make use of the Wannier basis defined in (5) to write the (N-particle) wave function as:

$$\psi(\boldsymbol{x};\boldsymbol{a}) = \langle \boldsymbol{x},\boldsymbol{a}|\psi\rangle\,. \tag{23}$$

We can switch back to to second quantization with

$$|\psi\rangle = \frac{1}{N!}\sum_{x_1\ldots x_N=1}^{L}\sum_{a_1\ldots a_N=\uparrow,\downarrow}\psi(\boldsymbol{x};\boldsymbol{a})\,|\boldsymbol{x},\boldsymbol{a}\rangle\,. \tag{24}$$

Knowing this, we can express the Schrödinger equation as $\langle \boldsymbol{x},\boldsymbol{a}|H|\psi\rangle = E\psi(\boldsymbol{x};\boldsymbol{a})$. Now, how does the Hubbard Hamiltonian (2) act on the wannier states $|\boldsymbol{x},\boldsymbol{a}\rangle$? Using the commutation relations (3) and (4) and introducing the row vectors $\boldsymbol{e}^\alpha, \alpha \in \{1,\ldots,N\}$ which have zeros everywhere except for column α, where they have a one:

$$\begin{aligned} H\,|\boldsymbol{x},\boldsymbol{a}\rangle &= \left(-\sum_{j=1}^{L}\sum_{a=\uparrow,\downarrow}\left(c^\dagger_{j,a}c_{j+1,a} + c^\dagger_{j+1,a}c_{j,a}\right) + 4u\sum_{j=1}^{L} n_{j\uparrow}n_{j\downarrow}\right)|\boldsymbol{x},\boldsymbol{a}\rangle \\ &= -\sum_{j=1}^{N}(|(\boldsymbol{x}-\boldsymbol{e}^j) \bmod L,\boldsymbol{a}\rangle + |(\boldsymbol{x}+\boldsymbol{e}^j) \bmod L,\boldsymbol{a}\rangle) \\ &\quad + 4u\sum_{1\le k<l\le N}\delta_{x_k,x_l}\,|\boldsymbol{x},\boldsymbol{a}\rangle\,, \end{aligned} \tag{25}$$

where for the hopping part of (2), say H_0, we used that $[c^\dagger_{j,a}c_{j\pm1,a}, c^\dagger_{k,b}] = c^\dagger_{j,a}\{c_{j\pm1,a}, c^\dagger_{k,b}\} = \delta_{j\pm1,k}\delta_{a,b}c^\dagger_{j,a}$ and the periodic boundary conditions $c^\dagger_{0,b} = c^\dagger_{L,b}$, $c^\dagger_{L+1,b} = c^\dagger_{1,b}$ imply $[H_0, c^\dagger_{x_j,b}] = -c^\dagger_{x_j-1,b} - c^\dagger_{x_j+1,b}$. Using this we can calculate

$$\langle \boldsymbol{x},\boldsymbol{a}|H|\psi\rangle = -\sum_{j=1}^{N}(\Delta^-_{j,L}\psi(\boldsymbol{x};\boldsymbol{a}) + \Delta^+_{j,L}\psi(\boldsymbol{x};\boldsymbol{a})) + 4u\sum_{1\le k<l\le N}\delta_{x_k,x_l}\psi(\boldsymbol{x};\boldsymbol{a}) \tag{26}$$

where we defined cyclic shift operators for one particle:

$$\Delta^\pm_{j,L}\psi(\boldsymbol{x};\boldsymbol{a}) = \psi((\boldsymbol{x}\pm\boldsymbol{e}^j) \bmod L;,\boldsymbol{a}). \tag{27}$$

Now one can express the Schrödinger equation in the more convenient coordinate representation:

$$H_N^{(L)}\psi(\boldsymbol{x};\boldsymbol{a}) = E\psi(\boldsymbol{x};\boldsymbol{a}) \tag{28}$$

defining the N particle Hubbard Hamiltonian

$$H_N^{(L)} = -\sum_{j=1}^{N}(\Delta_{j,L}^{-} + \Delta_{j,L}^{+}) + 4u \sum_{1\leq k<l\leq N} \delta_{x_k,x_l}. \tag{29}$$

Similarly we can write $\hat{U}$ in coordinate form, starting from equation (11):

$$\langle \boldsymbol{x},\boldsymbol{a}|\hat{U}|\psi\rangle = \prod_{j=1}^{N}\Delta_{j,L}^{+}\psi(\boldsymbol{x};\boldsymbol{a}) \implies \hat{U}_N^{(L)}\psi(\boldsymbol{x};\boldsymbol{a}) = \omega\psi(\boldsymbol{x};\boldsymbol{a}) \tag{30}$$

where $\hat{U}_N^{(L)} = \prod_{j=1}^{N}\Delta_{j,L}^{+}$. The equations (28) and (30) are still too hard too solve because of the implied cyclic property of the equations. We can therefore better let the length of the lattice go to infinity and afterwards impose boundary conditions. To do this we introduce non-cyclic operators:

$$\Delta_j^{\pm}\psi(\boldsymbol{x};\boldsymbol{a}) = \psi(\boldsymbol{x}\pm\boldsymbol{e}^j;\boldsymbol{a}) \tag{31}$$

$$H_N = -\sum_{j=1}^{N}(\Delta_j^{-} + \Delta_j^{+}) + 4u \sum_{1\leq k<l\leq N} \delta_{x_k,x_l} \tag{32}$$

$$\hat{U}_N = \prod_{j=1}^{N}\Delta_j^{+}. \tag{33}$$

Such that the equations we need to solve become

$$H_N\psi(\boldsymbol{x};\boldsymbol{a}) = E\psi(\boldsymbol{x};\boldsymbol{a}) \tag{34}$$

$$\hat{U}_N\psi(\boldsymbol{x};\boldsymbol{a}) = \omega\psi(\boldsymbol{x};\boldsymbol{a}), \tag{35}$$

where the shift operators $\Delta_j^{\pm}$ are subject to the periodic boundary conditions:

$$(\Delta_j^{\pm} - \Delta_{j,L}^{\pm})\psi(\boldsymbol{x};\boldsymbol{a}). \tag{36}$$

Solutions of (34) and (35) that satisfy (36) are also solutions of (28) and (30), but it turns out this is not true the other way around, as we will later see. Finding a solution to (34) and (35) is certainly no easy task. A full derivation of the solution in the Bethe ansatz method is very complicated and rather lengthy, for this I refer the reader to [7]. Therefore we will solve it not for N particles but for just $N = 2$ to illustrate the way this is done. Doing this is useful because one can still get a good insight into solving this problem with the Bethe ansatz method and see the Lieb-Wu equations for the two-particle case, where we can solve everything exactly fairly easily.

2.2 Solving the two-particle problem

For the two particle case the equations (34) and (35) become:

$$H_2\psi(x_1, x_2; a_1, a_2) = E\psi(x_1, x_2; a_1, a_2) \tag{37}$$

$$\hat{U}_2\psi(x_1, x_2; a_1, a_2) = \omega\psi(x_1, x_2; a_1, a_2) \tag{38}$$

where we have the two particle Hamiltonian and shift operator

$$H_2 = -(\Delta_1^+ + \Delta_1^- + \Delta_2^+ + \Delta_2^-) + 4u\delta_{x_1,x_2} \tag{39}$$

$$.\hat{U}_2 = \Delta_1^+\Delta_2^+ \tag{40}$$

Now the crucial step is to separate variables: the delta potential term in the hamiltonian only depends on the relative coordinate $n = x_1 - x_2$, so it makes sense to introduce, together with the relative coordinate, the center of mass coordinate $m = x_1 + x_2$ and make the assumption:

$$\psi(x_1, x_2; a_1, a_2) = f(m)g(n), \tag{41}$$

where f and g can depend on spin variables. Plugging this in (37) we get

$$\frac{f(m+1) + f(m-1)}{f(m)} = \frac{(4u\delta_{n,0} - E)g(n)}{g(n+1) + g(n-1)}. \tag{42}$$

So we get two linear difference equations with constant coefficients:

$$f(m+1) + f(m-1) = Cf(m) \tag{43}$$

$$g(n+1) + g(n-1) = \frac{4u\delta_{n,0} - E}{C}g(n), \tag{44}$$

where C is an undetermined constant. The solution to the equation (43) is a linear combination of:

$$f(m) = A^+w^m + A^-w^{-m}. \tag{45}$$

If we insert this back into (43) we see that $w + \frac{1}{w} = C$. Plugging it into (40) we get

$$f(m+2) = \omega f(m) \tag{46}$$

which implies that either A^+ or A^- is zero for $w \neq 1$, so f only depends on one (maybe spin dependent) amplitude (say A^+), which we absorb into g and we are left over with

$$f(m) = w^m, \tag{47}$$

$$\omega = w^2. \tag{48}$$

Now, for the g part we have again a general solution that after plugging back in (44) reads

$$g(n) = \begin{cases} A^{-+}z^n - A^{--}z^{-n} & \text{if } n < 0 \\ A^{++}z^n - A^{+-}z^{-n} & \text{if } n > 0 \end{cases} \tag{49}$$

where (44) for the energy reads:

$$E = -C(z + \frac{1}{z}) = -(w + \frac{1}{w})(z + \frac{1}{z}) \tag{50}$$

where in (49) there are some undetermined amplitudes $A^{\alpha\beta}$ with $\alpha, \beta \in \{+, -\}$ that depend on the spin variables of ψ. There are multiple constraining equations on these variables, beginning with consistency of g at $n = 0$. This gives

$$A^{+-} + A^{-+} = A^{++} + A^{--}, \tag{51}$$

which is the first constraint on $A^{\alpha\beta}$. Plugging $n = 0$ into (44) we get

$$(w + \frac{1}{w})(g(1) + g(-1)) = (4u - E)g(0) \tag{52}$$

$$\frac{1}{2}(wz - \frac{1}{wz} - \frac{w}{z} + \frac{z}{w})(A^{+-} + A^{++} - A^{-+} - A^{--}) = 4u(A^{-+} - A^{--}). \tag{53}$$

Now we introduce the important variables k_1 and k_2 and define s_j:

$$e^{ik_1} \equiv wz, \quad e^{ik_2} \equiv \frac{w}{z}, \quad s_j = \sin k_j, \quad j \in \{1, 2\}. \tag{54}$$

Notice that from this definition we have

$$w^m z^n = e^{i(k_1 x_1 + k_2 x_2)}, \quad w^m z^{-n} = e^{i(k_1 x_2 + k_2 x_1)}, \tag{55}$$

which will come in handy later. Using these definitions, equation (53) turns into the more elegant

$$(s_1 - s_2)(A^{+-} + A^{++} - A^{-+} - A^{--}) = 4iu(A^{-+} - A^{--}). \tag{56}$$

Now we want to impose more restrictions on the spin amplitudes such that we can fully determine g as a function of n, a_1 and a_2. The spin dependency lies fully in the spin amplitudes and therefore we can think of them as spinors with two indices: $A^{\alpha\beta}_{a_1 a_2}$. In the next steps we need a permutation matrix which swaps the indices of the spin amplitudes: $\Pi^{b_1 b_2}_{a_1 a_2} = \delta^{b_1}_{a_2}\delta^{b_2}_{a_1}$ such that

$$(\Pi A^{\alpha\beta})_{a_1 a_2}) = \sum_{b_1, b_2} \Pi^{b_1 b_2}_{a_1 a_2} A^{\alpha\beta}_{b_1 b_2} = A^{\alpha\beta}_{a_2 a_1}. \tag{57}$$

We then remember that we are dealing with electrons, so the wavefunction must be totally anti-symmetric under exchanging $x_1 \leftrightarrow x_2$, which corresponds to

$n \mapsto -n$, while also $a_1 \leftrightarrow a_2$. Thus the following must hold: $g(n) = -\Pi g(-n)$, because only g in ψ depends on n and the spin. What follows is

$$A^{+-} = \Pi A^{-+}, \tag{58}$$

$$A^{++} = \Pi A^{--}. \tag{59}$$

We now have four different equations for four different variables $A^{\alpha\beta}$ (namely, equations (51), (56), (58) and (59)), but there turns out to be just three independent ones. For the full derivation of the spin amplitudes I point the reader to Essler's book [7]. In the end we get the following formula for g, with just one spin amplitude A^{-+} remaining:

$$g(n) = \begin{cases} A^{-+}z^n - Y(s_1 - s_2)A^{-+}z^{-n} & \text{if } n \leq 0 \\ Y(s_1 - s_2)\Pi A^{-+}z^n - \Pi A^{-+}z^{-n} & \text{if } n \geq 0 \end{cases} \tag{60}$$

where the so called Yang's Y-operator (which acts on the spin amplitudes) is defined by

$$Y(\lambda) = \frac{2iu + \lambda\Pi}{2iu + \lambda} \tag{61}$$

Now we can find the full wave function (for $C \neq 0$) by inserting (47) and (60) into (41), while using (55):

$$\psi(x_1, x_2) = \begin{cases} A^{-+}e^{i(k_1x_1+k_2x_2)} - Y(s_1 - s_2)A^{-+}e^{i(k_1x_2+k_2x_1)} & \text{if } x_1 \leq x_2 \\ Y(s_1 - s_2)\Pi A^{-+}e^{i(k_1x_1+k_2x_2)} - \Pi A^{-+}e^{i(k_1x_2+k_2x_1)} & \text{if } x_1 \geq x_2 \end{cases} \tag{62}$$

for $C \neq 0$, which corresponds to $k_1, k_2 \in \mathbb{C}, k_1 + k_2 \neq \pi \bmod 2\pi$. A fun fact: this looks much like the original bethe ansatz state, whereas Bethe himself used a similar wavefunction as an ansatz depending on a linear combination of $e^{i(k_1x_1+k_2x_2)}$ and $e^{i(k_1x_2+k_2x_1)}$ (in the two particle case) to exactly solve the problem of the one-dimensional spin chain in 1931 [5]. Despite this great accomplishment at the time, it was not until some time later that other models (like the Hubbard model) were solved with the Bethe ansatz. Now let us carry on with the derivation. This makes the eigenvalues of the Hamiltonian and the shift operator equal to

$$E = -2\cos k_1 - 2\cos k_2 \tag{63}$$

$$\omega = e^{i(k_1+k_2)} \tag{64}$$

Now, what is the spin amplitude A^{-+}? It turns out to be a linear combination of spin singlet state ϕ_{sing} and the spin triplet state ϕ_{trip}, where

$$\phi_{sing}(a_1, a_2) = \delta_{a_1,\uparrow}\delta_{a_2,\downarrow} - \delta_{a_1,\downarrow}\delta_{a_2,\uparrow} \tag{65}$$

$$\phi_{trip}(a_1, a_2) = \begin{cases} \delta_{a_1,\uparrow}\delta_{a_2,\uparrow} \\ \delta_{a_1,\uparrow}\delta_{a_2,\downarrow} + \delta_{a_1,\downarrow}\delta_{a_2,\uparrow} \\ \delta_{a_1,\downarrow}\delta_{a_2,\downarrow} \end{cases} . \tag{66}$$

Equipped with this and

$$\Pi\phi_{sing} = -\phi_{sing}, \quad \Pi\phi_{trip} = \phi_{trip} \tag{67}$$

we can write the singlet solution as

$$\psi(x_1, x_2) = \phi_{sing} \cdot \begin{cases} e^{i(k_1x_1+k_2x_2)} + \frac{s_1-s_2-2iu}{s_1-s_2+2iu} e^{i(k_1x_2+k_2x_1)} & \text{if } x_1 \leq x_2 \\ \frac{s_1-s_2-2iu}{s_1-s_2+2iu} e^{i(k_1x_1+k_2x_2)} + e^{i(k_1x_2+k_2x_1)} & \text{if } x_1 \geq x_2 \end{cases} \tag{68}$$

and the triplet solution as

$$\psi(x_1, x_2) = \phi_{trip} \cdot (e^{i(k_1x_1+k_2x_2)} - e^{i(k_1x_2+k_2x_1)}). \tag{69}$$

2.3 From boundary conditions to Lieb-Wu equations

Okay, great! Finally we got solutions (68) and (69) to the equations (34) and (35), which look like two scattering electrons in either a singlet or triplet state, in position x_1 and x_2 and with momentum k_1 and k_2, respectively (which of course, makes sense). But we still have to impose the boundary conditions (36). These can be summarized as

$$\psi(0, x_2; \boldsymbol{a}) = \psi(L, x_2; \boldsymbol{a}), \quad \psi(L+1, x_2; \boldsymbol{a}) = \psi(1, x_2; \boldsymbol{a}) \tag{70}$$

(and similarly for x_2). If we now fill in our general solution (62) into (70) we get

$$\begin{aligned} &e^{ik_1L} \left(Y(s_1-s_2)\Pi - e^{-ik_1L}\right) A^{-+} e^{ik_2x_2} \\ &- e^{ik_2L} Y(s_1-s_2) \left(Y(s_2-s_1)\Pi - e^{-ik_2L}\right) A^{-+} e^{ik_1x_2} = 0 \end{aligned} \tag{71}$$

where we used $Y(\lambda)Y(-\lambda) = 1$ and $x_2 \in \{1, \ldots, L\}$. If $k_1 \neq k_2$ then e^{ik_1L} and e^{ik_2L} are linearly independent and the following is therefore necessary and sufficient:

$$Y(s_1-s_2)\Pi A^{-+} = e^{-ik_1L} A^{-+} \tag{72}$$

$$Y(s_2-s_1)\Pi A^{-+} = e^{-ik_1L} A^{-+}. \tag{73}$$

Then for the singlet state ϕ_{sing}, using (61) and (67):

$$e^{ik_1L} = \frac{s_1-s_2+2iu}{s_1-s_2-2iu}, \quad e^{ik_2L} = \frac{s_2-s_1+2iu}{s_2-s_1-2iu}. \tag{74}$$

For the triplet state ϕ_{trip}, again using (61) and (67):

$$e^{ik_1L} = e^{ik_2L} = 1. \tag{75}$$

The last equations (74) and (75) can be interpreted as the Lieb-Wu equations $N = 2$ and $M = 1$, where M is the number of down spin electrons. We will generalize this formula to the N-particle case, but firstly we will not get away

without discussing what happened to the $C = 0$ case. Here we still have (47) together with $w^2 = -1$ to get $f(m) = (\pm i)^m$ and for g we have

$$(4u\delta_{n,0} - E)g(n) = 0 \tag{76}$$

which has two different non-trivial solutions: $E = 0$ and $E = 4u$. In the first case everything is pretty much the same, again with the anti-symmetric wave function given by (62) but now with *arbitrary* $k_1, k_2 \in \mathbb{C}$. The other possibility gives us a more interesting solution, which is $g(n) = A\delta_{n,0}$. Again we require

$$g(n) = -\Pi g(-n) \implies \Pi A = -A \tag{77}$$

which means $A = \phi_{sing}$ such that $g(n) = \phi_{sing}\delta_{n,0}$ and the wavefunction becomes

$$\psi(x_1, x_2) = \phi_{sing}(-1)^{x_1}\delta_{x_1,x_2}. \tag{78}$$

This looks like a weird solution: it is a bound state of two electrons even though their interaction can be repulsive ($U > 0$). We also see that this state does *not* satisfy our boundary equations because it is not a solution to (70) ($\psi(0, L) = 0 \neq \psi(L, L) = \phi_{sing}(-1)^L$). Still, it *is* an eigenstate of the cyclic two-particle Hamiltonian and the two-particle shift operator (equations (28) and (30) for $N = 2$): $(H_2^{(L)}\psi)(x_1, x_2) = 4u\psi(x_1, x_2)$. Therefore, as we mentioned, there are some solutions of (28) and (30) which are not solutions of (34) and (35) with the boundary conditions (36). Is this a problem? It turns out that here the SO(2) symmetry of the η-pairs comes into play. If we use (24) to switch back to second quantization of the wavefunction (78), we get:

$$|\psi\rangle = \frac{1}{2}\sum_{x_1,x_2=1}^{L}\sum_{a_1a_2=\uparrow,\downarrow}\psi(\boldsymbol{x};\boldsymbol{a})\,|\boldsymbol{x},\boldsymbol{a}\rangle \tag{79}$$

$$= \frac{1}{2}\sum_{x_1,x_2=1}^{L}\sum_{a_1a_2=\uparrow,\downarrow}(-1)^{x_1}\delta_{x_1,x_2}\left(\delta_{a_1,\uparrow}\delta_{a_2,\downarrow} - \delta_{a_1,\downarrow}\delta_{a_2,\uparrow}\right)c^\dagger_{x_2,a_2}c^\dagger_{x_1,a_1}\,|0\rangle \tag{80}$$

$$= \sum_{x_1=1}^{L}(-1)^{x_1}c^\dagger_{x_1,\downarrow}c^\dagger_{x_1,\uparrow}\,|0\rangle = \eta^+\,|0\rangle\,, \tag{81}$$

where we used equation (17) for η^+. Therefore we can get this state out of the solutions of the Bethe ansatz method by applying η-symmetry operators to them. This is generalized to the N particle case. The Bethe ansatz wavefunctions that one gets after a lengthy calculation (see, for example, [7]) will be either the lowest or highest weight states of the symmetry (either spin or η) operators. We can get the full spectrum of the cyclic Hamiltonian and shift operator by applying these symmetry operators on them.
These Bethe ansatz states, which are thus eigenfunctions of the N-particle infinite interval Hamiltonian (34) and shift operator (35) subject to the boundary condition (36), for N electrons and M down spins, are specified by two sets of

quantum numbers: $k_j,\ j \in \{1,\dots,N\}$ and $\lambda_l,\ l \in \{1,\dots,M\}$, $2M \leq N \leq L$. We call the k_j charge momenta and λ_l spin rapidities and we group them into row vectors: $\boldsymbol{k} = (k_1,\dots,k_N)$, $\boldsymbol{\lambda} = (\lambda_1,\dots,\lambda_M)$, so we can act on them with elements from the symmetric group of order N (or M) $\mathfrak{S}^N$, wherefore I assume the reader is familiar. An element $Q \in \mathfrak{S}^N$ acts on the vectors as $\boldsymbol{k}Q = (k_{Q(1)},\dots,k_{Q(N)})$. It turns out the wavefunctions depend on the order of the positions of the electrons, x_j. For a specific ordering $Q \in \mathfrak{S}^N$:

$$1 \leq x_{Q(1)} \leq \cdots \leq x_{Q(N)} \leq L. \tag{82}$$

For this ordering, the Bethe ansatz wavefunctions are given by:

$$\psi(\boldsymbol{x};\boldsymbol{a}|\boldsymbol{k};\boldsymbol{\lambda}) = \sum_{P\in\mathfrak{S}^N} \operatorname{sign}(PQ)\,\langle \boldsymbol{a}Q|\boldsymbol{k}P,\boldsymbol{\lambda}\rangle\, e^{i\langle \boldsymbol{k}P,\boldsymbol{x}Q\rangle} \tag{83}$$

where

$$\langle \boldsymbol{a}Q|\boldsymbol{k}P,\boldsymbol{\lambda}\rangle = \sum_{R\in\mathfrak{S}^M} A(\boldsymbol{\lambda}R)\prod_{l=1}^{M} F_{\boldsymbol{k}P}(\lambda_{R(l)};y_l) \tag{84}$$

$$F_{\boldsymbol{k}}(\lambda;y) = \frac{2iu}{\lambda-\sin k_y+iu}\prod_{j=1}^{y-1}\frac{\lambda-\sin k_j-iu}{\lambda-\sin k_j+iu} \tag{85}$$

$$A(\boldsymbol{\lambda}) = \prod_{1\leq m<n\leq M}\frac{\lambda_m-\lambda_n-2iu}{\lambda_m-\lambda_n} \tag{86}$$

where the y_j are the coordinates of the jth down spin of the $a_{Q(1)},\dots,a_{Q(N)}$ sequence. Okay, phew... Now, the only things left to calculate are the charge momenta k_j and the spin rapidities λ_l, which is done imposing the periodic boundary conditions through (finally) the Lieb-Wu equations:

$$e^{ik_jL} = \prod_{l=1}^{M}\frac{\lambda_l-\sin k_j-iu}{\lambda_l-\sin k_j+iu}, \quad j=1,\dots,N, \tag{87}$$

$$\prod_{j=1}^{N}\frac{\lambda_l-\sin k_j-iu}{\lambda_l-\sin k_j+iu} = \prod_{\substack{m=1\\m\neq l}}^{M}\frac{\lambda_l-\lambda_m-2iu}{\lambda_l-\lambda_m+2iu} \quad l=1,\dots,M. \tag{88}$$

After all this, the Bethe ansatz wavefunctions (83) are eigenfunctions of the Hamiltonian (34) and the momentum operator, which is a function of the shift operator (35), with eigenvalues

$$E = -2\sum_{j=1}^{N}\cos k_j + u(L-2N), \quad P = \left[\sum_{j=1}^{N} k_j\right] \bmod 2\pi. \tag{89}$$

3 String solutions

The solutions, also known as the roots, of the Lieb-Wu equations as given by (87) and (88) are in general quite hard to find, even numerically. But once one

looks at the thermodynamic limit they are actually relatively easy to find. The numbers k and λ can in general be assumed to be complex numbers. It so happens that these numbers are found in strings of solutions: a set of solutions for the roots is (almost) regularly spaced in the complex plane. From those strings, one can find solutions involving only the real part of the roots. This is known as the string hypothesis [5]. The string solutions of the Hubbard model were first found by Takahashi in 1972 [10].
From the solutions on these strings actually all 4^L solutions can be found by applying the lowering operators of the spin and raising operators of the η-spin, as was shown by Essler, Korepin and Schoutens [11]. This is because the solutions that are found by the string hypothesis are the highest and lowest weight solutions of the spin and η-spin operators respectively. We will only work with the thermodynamic limit, so these solutions will be valid.

3.1 $k - \Lambda$ strings and Λ strings

Let us now actually turn to finding the solutions. Start by assuming that L is very large and k_j has a non-zero complex part for some j. This means that the exponential on the left of equation (87) blows up for this k_j. Therefore on the right side at least one of the factors must be very close to a pole. This condition can then be substituted in another Lieb-Wu equation and one can repeat this, until there are as many simplified equations as unknown variables, at which point the solutions can be found, giving $2m$ k's and m Λ's that combine into a $k - \Lambda$ string of length $2m$.
For the simplest example where $N = 2$ and $M = 1$ we can quickly do this by hand [7]. The Lieb-Wu equations (87) and (88) can then be written as

$$e^{ik_1 L} = \frac{\Lambda' - \sin k_1 - iu}{\Lambda' - \sin k_1 + iu} \tag{90}$$

$$e^{ik_2 L} = \frac{\Lambda' - \sin k_2 - iu}{\Lambda' - \sin k_2 + iu} \tag{91}$$

$$\frac{\Lambda' - \sin k_1 - iu}{\Lambda' - \sin k_1 + iu} \cdot \frac{\Lambda' - \sin k_2 - iu}{\Lambda' - \sin k_2 + iu} = 1, \tag{92}$$

where $k_1 = a - ib$, with $b > 0$ by assumption, such that equation (90) becomes exponentially large in the thermodynamic limit. We therefore have

$$\Lambda' = \sin k_1 - iu \tag{93}$$

$$\Rightarrow k_1 = \pi - \sin^{-1}(\Lambda' + iu) \tag{94}$$

to exponential precision. This then leads to the first factor in (92) being exponentially large, which in turn forces the second term to be exponentially close to zero. We therefore also have the equation

$$\Lambda' = \sin k_2 + iu \tag{95}$$

$$\Rightarrow k_2 = \pi - \sin^{-1}(\Lambda' - iu). \tag{96}$$

The last unknown Λ' can then be numerically found by eliminating k_1 and k_2 in (92) using (93) and (95) and specifying u. Then applying a root finding algorithm, one can find Λ'. This is the general way to go about these problems.
By using a similar trick and assuming λ_l to be complex, we find a second type of strings only involving the Λ's, known as Λ strings. If we assume all k_j to be real, then for large N and $M \ll N$, we see that the left hand side of equation (88) goes to zero, since the fraction is always less than one for every term. It must therefore be true that at least one of the right hand side terms is close to zero. This argument can then be repeated and one finds a Λ string of length m. These techniques can be generalized to find the string solutions for bigger systems than in our example. In general, a solution to the Lieb-Wu equations looks like a combination of several string solutions. We thus label the different strings by an index α. The solutions for a $k-\Lambda$ string of length $2m$ then become [10]

$$\begin{aligned}
k_\alpha^1 =& \pi - \sin^{-1}(\Lambda_\alpha'^m + miu),\\
k_\alpha^2 =& \sin^{-1}(\Lambda_\alpha'^m + (m-2)iu),\\
k_\alpha^3 =& \pi - k_\alpha^2,\\
&\vdots\\
k_\alpha^{2m-2} =& \sin^{-1}(\Lambda_\alpha'^m - (m-2)iu),\\
k_\alpha^{2m-1} =& \pi - k_\alpha^{2m-2},\\
k_\alpha^{2m} =& \pi - \sin^{-1}(\Lambda_\alpha'^m - miu),
\end{aligned} \tag{97}$$

$$\Lambda_\alpha'^{m,j} = \Lambda_\alpha'^m + (m-2j+1)iu, \quad j = 1, \ldots, m, \tag{98}$$

while the solutions of a Λ string are given by

$$\Lambda_\alpha^{m,j} = \Lambda_\alpha^m + (m-2j+1)iu, \quad j = 1, \ldots, m. \tag{99}$$

Here, Λ_α^m are the real centers of the string. Also note the difference between the primed and unprimed Λ's, distinguishing between Λ's found from $k-\Lambda$ strings and Λ strings respectively.
One may wonder what the physical significance of these complex solutions is, since plane waves are given by real k_j's. One can show that for complex k_j's the wave function describes a bound state: the wave function decays exponentially as a function of the distance in coordinates between electrons [7, 11]. We are, however, generally more interested in plane wave solutions, and thus in real-valued $k_j's$. We will elaborate on this in the following section.

3.2 Takahashi's equations

Summarizing our last section, there are three types of solutions. We have

- M_n Λ strings of length n;
- M_n' $k-\Lambda$ strings of length n;

- M_e single k_j's.

These strings satisfy

$$M = \sum_{n=1}^{\infty} n(M_n + M'_n), \tag{100}$$

$$N = M_e + \sum_{n=1}^{\infty} 2nM'_n, \tag{101}$$

with N the number of particles and M the number of down spins, as before. We see that this is indeed true if each k_j describes an electron, while each λ describes an electron with spin down. These equations let us rewrite the first Lieb-Wu equations (87) into

$$e^{ik_jL} = \prod_{n,m,\alpha} \frac{\Lambda_\alpha^{n,m} - \sin k_j - iu}{\Lambda_\alpha^{n,m} - \sin k_j + iu} \prod_{n,m,\alpha} \frac{\Lambda_\alpha'^{n,m} - \sin k_j - iu}{\Lambda_\alpha'^{n,m} - \sin k_j + iu}, \tag{102}$$

after which we can fill in equations (98) and (99), which were the solutions for the Λ's [10]. We then see that most terms of the products in m can be crossed out, since the denominator of one term is the same as the numerator of the next and only the outer two terms remain, giving

$$e^{ik_jL} = \prod_{n,\alpha} \frac{\Lambda_\alpha^{n} - \sin k_j - inu}{\Lambda_\alpha^{n} - \sin k_j + inu} \prod_{m,n,\alpha} \frac{\Lambda_\alpha'^{n} - \sin k_j - inu}{\Lambda_\alpha'^{n} - \sin k_j + inu} \tag{103}$$

Taking the logarithm then gives

$$k_jL = 2\pi I_j - \sum_{n=1}^{\infty} \sum_{\alpha=1}^{M_n} \theta\left(\frac{\sin k_j - \Lambda_\alpha^n}{nu}\right) - \sum_{n=1}^{\infty} \sum_{\alpha=1}^{M'_n} \theta\left(\frac{\sin k_j - \Lambda_\alpha'^n}{nu}\right), \tag{104}$$

where $\theta(x) = 2\arctan(x)$ and

$$I_j \text{ is } \begin{cases} \in \mathbb{Z} & \text{if } \sum_m (M_m + M'_m) \text{ is even} \\ \in \mathbb{Z} + \frac{1}{2} & \text{if } \sum_m (M_m + M'_m) \text{ is odd} \end{cases} \tag{105}$$

are the branches of the log and we used that

$$\ln\left(\frac{1 - xi}{1 + xi}\right) = -2i\arctan(x).$$

These I_j are limited by the invariance of a 2π phase shift of the complex exponential in (103) and are thus given within the range

$$-\frac{L}{2} \leq I_j \leq \frac{L}{2}. \tag{106}$$

For the second Lieb-Wu equation we can do something similar, but these steps are a bit more involved and will not be given here. The result is given by the following two equations, which are the second and third Takahashi equations,

$$\sum_{j=1}^{N-2M'} \theta\left(\frac{\Lambda_\alpha^n - \sin k_j}{nu}\right) = 2\pi J_\alpha^n + \sum_{m=1}^{\infty}\sum_{\beta=1}^{M_m} \Theta_{nm}\left(\frac{\Lambda_\alpha^n - \Lambda_\beta^m}{u}\right) \tag{107}$$

$$\begin{aligned} 2L\,\mathrm{Re}(\arcsin(\Lambda_\alpha'^n + inu)) = 2\pi J_\alpha'^n &+ \sum_{j=1}^{N-2M'} \theta\left(\frac{\Lambda_\alpha'^n - \sin k_j}{nu}\right) \\ &+ \sum_{m=1}^{\infty}\sum_{\beta=1}^{M_m'} \Theta_{nm}\left(\frac{\Lambda_\alpha'^n - \Lambda_\beta'^m}{u}\right) \end{aligned} \tag{108}$$

where we've defined $M' = \sum_n nM_n'$ as the total number of Λ's in $k-\Lambda$ strings. The function Θ_{nm} is given by

$$\Theta_{nm}(x) = \begin{cases} \theta\left(\frac{x}{|n-m|}\right) + 2\theta\left(\frac{x}{|n-m|+2}\right) + \ldots + 2\theta\left(\frac{x}{n+m-2}\right) + \theta\left(\frac{x}{n+m}\right) & \text{if } n \neq m \\ 2\theta\left(\frac{x}{2}\right) + 2\theta\left(\frac{x}{4}\right) + \ldots + 2\theta\left(\frac{x}{2n-2}\right) + 2\theta\left(\frac{x}{2n}\right) & \text{if } n = m \end{cases} \tag{109}$$

and J_α^n and $J_\alpha'^n$ again label the different branches of the logarithm and are given by

$$J_\alpha^n \text{ is } \begin{cases} \in \mathbb{Z} & \text{if } N - M_n \text{ is odd} \\ \in \mathbb{Z} + \frac{1}{2} & \text{if } N - M_n \text{ is even,} \end{cases} \tag{110}$$

$$J_\alpha'^n \text{ is } \begin{cases} \in \mathbb{Z} & \text{if } L - N + M_n' \text{ is odd} \\ \in \mathbb{Z} + \frac{1}{2} & \text{if } L - N + M_n' \text{ is even,} \end{cases} \tag{111}$$

with ranges

$$|J_\alpha^n| \leq \frac{1}{2}\left(N - 2M' - \sum_{m=1}^{\infty} t_{mn}M_m - 1\right), \tag{112}$$

$$|J_\alpha'^n| \leq \frac{1}{2}\left(L - N + 2M' - \sum_{m=1}^{\infty} t_{mn}M_m' - 1\right) \tag{113}$$

that are similar to the ones found by Yang & Yang for a different model [12]. Here t_{mn} is defined as

$$t_{mn} = 2\min(m,n) - \delta_{mn}. \tag{114}$$

The numbers I_j, J_α^n and $J_\alpha'^n$ are equivalent to our original roots of the Lieb-Wu equations k_j, Λ_α^n and $\Lambda_\alpha'^n$ in the sense that every set of quantum numbers $\{I_j, J_\alpha^n, J_\alpha'^n\}$ determines a unique solution that is an eigenfunction of the Hubbard Hamiltonian. It is thus equally valid to describe our system in these quantum numbers, which gives a more intuitive picture, equivalent to the one shown in class. See for example figure 1, where a possible configuration of quantum numbers is given.

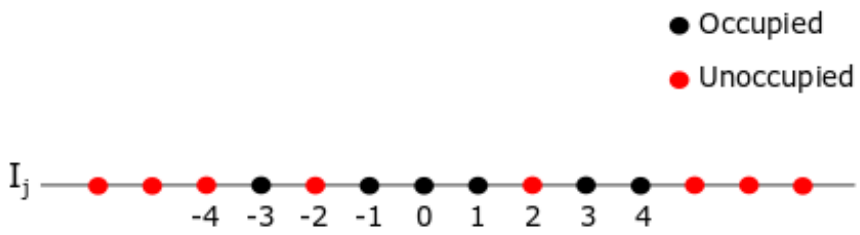

Figure 1: A possible configuration of quantum numbers I_j, describing some excited state of the Hubbard model with 6 electrons. We've chosen $\sum_m (M_m + M'_m)$ even, such that all I_j are integer.

4 The thermodynamic Bethe Ansatz

We can now start to apply the solutions we found to extract some physical properties from our system. For Takahashi's equations (104), (107) and (108) one can define so called counting functions $y(k)$, $z_n(\Lambda)$ and $z'_n(\Lambda')$ as follows [7]

$$Ly(k) = kL + \sum_{n=1}^{\infty}\sum_{\alpha=1}^{M_n}\theta\left(\frac{\sin k - \Lambda_\alpha^n}{nu}\right) + \sum_{n=1}^{\infty}\sum_{\alpha=1}^{M'_n}\theta\left(\frac{\sin k - \Lambda_\alpha'^n}{nu}\right), \tag{115}$$

$$Lz_n(\Lambda) = \sum_{j=1}^{N-2M'}\theta\left(\frac{\Lambda - \sin k_j}{nu}\right) - \sum_{m=1}^{\infty}\sum_{\beta=1}^{M_m}\Theta_{nm}\left(\frac{\Lambda - \Lambda_\beta^m}{u}\right), \tag{116}$$

$$\begin{aligned} Lz'_n(\Lambda') = {} & L(\arcsin(\Lambda' + niu) + \arcsin(\Lambda' - niu)) \\ & - \sum_{j=1}^{N-2M'}\theta\left(\frac{\Lambda' - \sin k_j}{nu}\right) - \sum_{m=1}^{\infty}\sum_{\beta=1}^{M_m}\Theta_{nm}\left(\frac{\Lambda' - \Lambda_\beta^m}{u}\right), \end{aligned} \tag{117}$$

which are constructed in such a way that

$$y(k_j) = \frac{2\pi I_j}{L}, \quad z_n(\Lambda_\alpha^n) = \frac{2\pi J_\alpha^n}{L}, \quad z'_n(\Lambda_\alpha'^n) = \frac{2\pi J_\alpha'^n}{L}. \tag{118}$$

In the thermodynamic limit we can also define root densities as a generalization of giving all the roots. We can define particle- and hole-like densities for k as $\rho^p(k)$ and $\rho^h(k)$ respectively and similarly for $\Lambda^{(\prime)}$ we define $\sigma^{(\prime)p}(\Lambda^{(\prime)})$ and $\sigma^{(\prime)h}(\Lambda^{(\prime)})$. Takahashi's equations can then be written in integral form, using these densities and the counting functions defined in equations (115)-(117). We will not give the derivation here, since it is rather involved and we would like to get to some actual thermodynamic properties of the system. The integral

formulas are given by [7, 10]:

$$\rho^p(k) + \rho^h(k) = \frac{1}{2\pi} + \cos(k) \sum_{n=1}^{\infty} \int_{-\infty}^{\infty} \mathrm{d}\Lambda a_n(\Lambda - \sin k)(\sigma_n'^p(\Lambda) + \sigma_n^p(\Lambda)) \quad (119)$$

$$\sigma_n^h(\Lambda) = -\sum_{m=1}^{\infty} A_{nm} * \sigma_m'^p \Big|_{\Lambda} + \int_{-\pi}^{\pi} \mathrm{d}k a_n(\sin k - \Lambda)\rho^p(k), \quad (120)$$

$$\sigma_n'^h(\Lambda) = \frac{1}{\pi} \mathrm{Re}\, \frac{1}{\sqrt{1-(\Lambda - inu)^2}} - \sum_{m=1}^{\infty} A_{nm} * \sigma_m'^p \Big|_{\Lambda} - \int_{-\pi}^{\pi} \mathrm{d}k a_n(\sin k - \Lambda)\rho^p(k), \quad (121)$$

where

$$a_n(x) = \frac{1}{2\pi} \frac{2nu}{(nu)^2 + x^2}, \quad (122)$$

$$A_{nm} * f \Big|_x = \delta_{nm} f(x) + \int_{-\infty}^{\infty} \frac{\mathrm{d}y}{2\pi} \frac{\mathrm{d}}{\mathrm{d}x} \Theta_n m \left(\frac{x-y}{u} \right) f(y). \quad (123)$$

These equations thus describe exact solutions for the hole densities in terms of the particle densities in the thermodynamic limit.
We will now shortly discuss what happens to the ground state with no external magnetic field in the limit $U \to 0$. To do this, we first have to take a look at chemical potentials. It turns out that one can calculate chemical potentials by using the integral formulas (119)-(121) and defining the so called *dressed energies* which involve logarithms of the ratio of $\frac{\rho^h(k)}{\rho^p(k)}$ times the temperature T. Then we consider the *half-filled* model in the ground state, i.e. $T = 0$. Now something very interesting happens: one can easily see that for $U = 0$ in (2), the model describes free electrons on a lattice. This model is obviously a conducting one at half filling, since the electrons are free to move around. But now, if we very slightly turn on $U > 0$ by say a small ϵ, the Hubbard model spontaneously turns into an insulator! One can see this by looking at the jump in chemical potential at half filling. We denote the chemical potential μ_- for the energy difference of the half filled state and the almost half filled state:

$$\mu_-(u) = E(L, u) - E(L-1, u), \quad (124)$$

whereby the notation $E(N, u)$ we mean the ground state energy of the state with N electrons. By using the derivation of the particle densities and dressed energies mentioned above one will find for this chemical potential the following formula:

$$\mu_-(u) = 2 - 2u - 2\int_0^{\infty} \frac{\mathrm{d}\omega}{\omega} \frac{J_1(\omega)e^{-\omega u}}{\cosh \omega u}, \quad (125)$$

where J_n is the n-th Bessel function. Now we make use of the Shiba transformation (16), which tells us that $E(L-1, u) = E(L+1, u)$. The chemical potential

with one more electron, μ_+, is now given by

$$\mu_+(u) = E(L+1,u) - E(L,u) = -\mu_-(u) \tag{126}$$

$$\implies \mu_+ - \mu_- = -4 + 4u + 4\int_0^\infty \frac{\mathrm{d}\omega}{\omega} \frac{J_1(\omega)e^{-\omega u}}{\cosh \omega u}. \tag{127}$$

So we see that there is a gap in the potential at half filling given by (127). This means the model is an insulator for every non-zero $U(= 4ut)$. A transition from a metallic (conducting) to an insulating (non-conducting) phase is called a *Mott transition*. In the same paper where Lieb and Wu derived the Lieb-Wu equations to solve the Hubbard model exactly, they concluded that there is an absence of a Mott transition for non-zero U for the Hubbard model in one dimension [1].

5 Conclusion and Outlook

In this digest we have examined the Hubbard model, a model describing fermions (electrons) on a one-dimensional lattice with a nearest-neighbor hopping term and an on-site interaction term. What turns out to be special about this one-dimensional model is that, despite its non-zero interaction terms, it yields an exact solution. That is, the problem of solving the Schrödinger equation is reduced to finding roots of the coupled *algebraic* Lieb-Wu equations (87), (88). These are very useful in the thermodynamic limit where they can be solved by looking at the distribution of roots in the complex plane. Then one can compute the physical properties of the system, where we highlighted the magnetic properties of the material. A strange phenomenon arised here: the system is metallic for only $U = 0$, while it is an insulator for any non-zero U. This means the insulating property of the system originates *only* from the electron-electron interaction.
As an outlook from this short digest one could look at many further applications of this exact solution of the Hubbard model, not just the conductivity. These include looking at other phase transitions, adding a external magnetic field or a chemical potential term in the Hamiltonian, looking at excited states, investigating other limits, etc. For all these Essler's book is a good reference to the interested reader [7]. There are also other ways of solving the Hubbard model, using a method called quantum inverse scattering. I can refer readers interested in this method to the book [13]. Overall the exact solution of the Hubbard model by Lieb and Wu was a real breaking point in this field. It induced many useful applications as an approximation to, for example, particles in periodic potentials and low temperatures and can explain certain properties, like magnetism and electronic properties, much better than other theories do.

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