The generalized $t$-$V$ model in one dimension

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Abstract. We develop a systematic strong coupling approach for studying an extended $t$-$V$ model with interactions of a finite range. Our technique is not based on the Bethe ansatz and is applicable to both integrable and non-integrable models. We illustrate our technique by presenting analytic results for the ground state energy (up to order $7$ in $t/V$), the current density and density-density correlations for integrable and non-integrable models with commensurate filling factors. We further present preliminary numerical results for incommensurate non-integrable models.

1. Introduction

Low-dimensional materials are of very high interest at present due to their exceptional electronic properties. Furthermore, the effects of interactions are enhanced in low dimensions, which leads to a variety of highly non-trivial quantum phases. In one spatial dimension, prime examples are the Luttinger liquid and the Mott insulating phase [1]. While low-energy properties of these phases are well described by effective field theory techniques, calculating the parameters of the effective theories from first principles is typically challenging. One well established and often used method is based on the Bethe ansatz, which, in principle, can provide an exact solution for integrable systems.

The main limitation of the Bethe ansatz is its rather limited applicability: it can only be applied to models of very high symmetry (as integrability implies an infinite number of conserved quantities). Generalizing Bethe-ansatz-based calculations to non-integrable systems does not seem possible.

In this work, we study a specific lattice model, the so-called $t$-$V$ model, which has both integrable and non-integrable regimes. A rather elegant way of investigating the infinite coupling limit of this model was developed in Ref. [2] and a family of Mott insulating phases was found. We use a variant of the strong coupling expansion [3], mainly used for the investigation of lattice field theories [4, 5, 6], to extend and generalize the results of Ref. [2] to large but finite couplings. Our method is insensitive to integrability (or the lack of it) and we obtain ground state properties of the model as a series in $t/V$ with minimal effort.

The rest of the paper is organized as follows. Firstly, we will present the model in question. Then, we will present the strong coupling expansion (SCE) as a general method for any quantum model. We will also investigate the generalized $t$-$V$ model for Mott insulator densities using SCE and compare the results to the previous work. Finally, we will conclude by sketching the future research into this subject.
2. Generalized $t$-$V$ model

The Hamiltonian of long-range $t$-$V$ model of fermions on a one-dimensional ring of size $L$ is as follows [2]:

\[ \hat{H} = -t \sum_{i=1}^{L} \left( \hat{c}_i \hat{c}_{i+1} + \text{h.c.} \right) + \sum_{i=1}^{L} \sum_{m=1}^{p} U_m \hat{n}_i \hat{n}_{i+m} \]  \hspace{1cm} (1)

where $\hat{c}_i$ is a fermionic operator on site $i$, $\hat{n}_i = \hat{c}_i \hat{c}^\dagger_i$ is a particle number operator, $p$ is the maximum range of interactions and $t$ and $U_m$ are kinetic and potential energies respectively. We use periodic boundary conditions. For the range $p = 1$, the model is integrable and equivalent to the XXZ Heisenberg model after a Jordan-Wigner transformation [7]. The model is non-integrable for $p > 1$. We assume that $U_m \lesssim \frac{U_{m-1} + U_{m+1}}{2}$, so that we are in the correct phase of the system, as described in Refs. [2, 8, 9]. Another assumption is that the kinetic energy term will always be very small, $t \ll U_m$, and thus we can rewrite the Hamiltonian as:

\[ \hat{H} = \hat{H}_0 + \lambda \hat{V} \]  \hspace{1cm} (2)

with $\hat{H}_0$ being the unperturbed Hamiltonian containing the potential energy, $\hat{V}$ -- perturbation (kinetic energy) and $\lambda = t$ is a small parameter.

3. Strong coupling expansion

In the article by Hamer [3], he introduced a method to truncate the basis according to how states were connected to the unperturbed initial subspace. The method is to reorder the basis (usually this is the computer basis), firstly writing the desired subspace of unperturbed states that we want to approximate (0th step), then states connected to them (1st step), then states connected to the 1st step states (2nd step) and so on. It is easy to see that this results in a tri-block-diagonal Hamiltonian. We truncate the basis to the step of our choice, resulting in smaller, truncated Hamiltonian, which will describe the full system up to a specific perturbation order. However, the truncated basis is still usually quite big, thus we will use an altered version of this method, commonly used in the investigations of the one-dimensional analogue of quantum electrodynamics -- the Schwinger model [4, 5, 6].

The method is as follows. Firstly, let us select the desired initial subspace of unperturbed states that we want to approximate. Usually that will be the ground state, but if one is interested in the temperature dependance, that could be first excited states, second excited states, etc. We will designate states in this subspace by $|0\rangle$, which means that we will treat it as a 0th step of our SCE.

Secondly, to create states of the next step in SCE, we will act with perturbation operator $\hat{V}$ on the states from previous step, $\hat{V} |n\rangle$. $\hat{V} |n\rangle$ will be, in general, a linear combination of states from orders $n-1$, $n$ and $n+1$. It will not include lower orders, because $\hat{V} |n\rangle$ is defined to not include orders higher than $n+1$, which means $\forall_{n>2} (m^2 |\hat{V} |n\rangle = 0$ and $\forall_{n<0} (n^2 |\hat{V} |n\rangle = 0$. This shows that the Hamiltonian in such a basis is tri-block-diagonal, as in the original Hamer method. To properly define states in order $n+1$, we have to separate states in $\hat{V} |n\rangle$ according to their unperturbed energy -- the states must be eigenstates of $\hat{H}_0$. Thus, in the end:

\[ \hat{V} |n\rangle = \sum_j C_j |n-1\rangle + \sum_k C_k |n^k\rangle + \sum_l |n+1\rangle \]  \hspace{1cm} (3)

where $C_j, C_k$ are normalization constants. The new states $|n+1\rangle$ are not yet orthonormal to each other and to the previous states. After Gramm-Schmidt orthonormalization they become:

\[ |n\rangle = C_{\tilde{n},j} |\tilde{n}\rangle - \sum_{m=1}^{n-1} \sum_{k=1}^{l_{\text{max}}(m)} C_{\tilde{n},j;m,k} |m\rangle - \sum_{k=1}^{n-1} C_{\tilde{n},j;n,k} |n^k\rangle \]  \hspace{1cm} (4)
where coefficient \( C_{\bar{n},j} \) is normalization and other coefficients include normalization and projection: \( C_{\bar{n},j;m,k} = C_{\bar{n},j}(m^k|\bar{n}^j) \).

If we continue this procedure infinitely long, we will not necessarily produce the full basis. Thus, there may be states that are not producible by this procedure, which we will call \(|\alpha\rangle\), and which will form, together with states \(|n^i\rangle\), an orthonormal non-truncated basis of the system. However, we can easily see that using (3) and then (4):

\[
\langle\alpha|\hat{V}|n^i\rangle = \langle\alpha| \left( \sum_j C_j|n-1^j\rangle + \sum_k C_k|n^k\rangle + \sum_l |\bar{n}+1^l\rangle \right) \]
\[
= \sum_j C_j \langle\alpha|n-1^j\rangle + \sum_k C_k \langle\alpha|n^k\rangle + \sum_l \frac{1}{C_{n+1,l}} \times \]
\[
\times \left( \langle\alpha|n+1^l\rangle + \sum_{r=1}^n \sum_{k=1}^{k_{\text{max}}(n)} C_{n+1,l,r;k} \langle\alpha|r^k\rangle + \sum_{k=1}^{l-1} C_{n+1,l;n+1,k} \langle\alpha|n+1^k\rangle \right) \]
\[
= 0
\]

This proves that states \(|\alpha\rangle\) are in fact part of a completely different subspace of the Hamiltonian than states \(|n^i\rangle\). Therefore, eigenvalues of the desired subspace that we will be approximating will not depend on \(|\alpha\rangle\) and neither will any averages over states from this subspace.

The Hamiltonian is now in the tri-block-diagonal form:

\[
\hat{H} = \begin{pmatrix}
\hat{E}_0 + \lambda \hat{V}_{00} & \lambda \hat{V}_{01} & 0 & 0 & \cdots \\
\lambda \hat{V}_{01}^T & \hat{E}_1 + \lambda \hat{V}_{11} & \lambda \hat{V}_{12} & 0 & \cdots \\
0 & \lambda \hat{V}_{12}^T & \hat{E}_2 + \lambda \hat{V}_{22} & \lambda \hat{V}_{23} & \cdots \\
0 & 0 & \lambda \hat{V}_{23}^T & \hat{E}_3 + \lambda \hat{V}_{33} & \cdots \\
\vdots & \vdots & \vdots & \ddots & \ddots \\
0 & & & & \text{Hamiltonian elements between states } |\alpha\rangle
\end{pmatrix}
\]

where \( \hat{V}_{n,m} \) are projections of \( \hat{V} \) between states \(|n^i\rangle\) and \(|m^j\rangle\) and \( \hat{E}_n \) are projections of \( \hat{H}_0 \) between states \(|n^i\rangle\). We can now use the standard degenerate perturbation theory to show which Hamiltonian elements contribute to the \( m \)-th order correction of the desired subspace. For small perturbation \( \lambda \) Hamiltonian can be written as:

\[
\hat{H} = \hat{H}_0 + \lambda \sum_n \mathbb{P}_n \hat{V} \mathbb{P}_n + \lambda^2 \sum_{n \neq n} \mathbb{P}_n \hat{V} \mathbb{P}_k \hat{V} \mathbb{P}_n + \cdots
\]

In general, \( m \)-th order correction will include matrices of the form:

\[
\mathbb{P}_n \hat{V} \mathbb{P}_k \mathbb{V} \mathbb{P}_k \mathbb{V} \mathbb{P}_k \cdots \mathbb{V} \mathbb{P}_n \mathbb{V} = \left\{ \begin{array}{ll}
\hat{V}_{n,n} & \text{if } m = n \\
\hat{V}_{n,n+1} & \text{if } m = n + 1 \\
\hat{V}^T_{n-1,n} & \text{if } m = n - 1 \\
0 & \text{otherwise}
\end{array} \right.
\]
Thus we can immediately conclude that for perturbation correction of order \( m \) we need the following matrices:

\[
\begin{align*}
\hat{E}_0 + \lambda \hat{V}_{00}, & \quad \lambda \hat{V}_{01}, & \quad \hat{E}_1 + \lambda \hat{V}_{11}, & \quad \ldots, & \quad \hat{E}_p + \lambda \hat{V}_{pp}, & \quad (\lambda \hat{V}_{p,p+1})
\end{align*}
\]

This means that in every step of Hamer’s procedure, by including more states in the Hamiltonian matrix, we increase the accuracy of the desired subspace of states by two perturbation orders. More strictly, in SCE step \( k \) we will have precision of ground state energies up to order \( 2k + 1 \).

### 4. Results and comparison

The method described above was used on the generalized \( t-V \) model with various Mott insulating densities (critical densities). For a Mott insulator the subspace of unperturbed ground states is very small [2] and the Hamiltonian can be diagonalized analytically.

#### 4.1. \( Q = 1/2 \) (half-filling), \( p = 1 \) (integrable), SCE step 3

The truncated Hamiltonian for this case is of dimension \( 16 \times 16 \), but for a very large system size \( L \) it can be separated into two equal subspaces of dimension \( 8 \times 8 \), which can be easily diagonalized. The condition for the system size is \( L > (2 \times \text{step} + 1)(p + 1) \). The ground state is therefore 2-fold degenerate and the ground state energy was calculated to be:

\[
E_0 = -\frac{L}{U} t^2 + \frac{L}{U^2} t^4 + \mathcal{O}(t^8)
\]

The density-density correlation functions \( N_m = \left\langle \sum_{i=1}^{L} \hat{n}_i \hat{n}_{i+m} \right\rangle \) were found to be:

\[
N_1 = \frac{L^2}{U^2} - 3LT^4 + \mathcal{O}(t^8) \quad (12) \quad N_3 = 2L \frac{t^2}{U^2} - 5LT^4 + \mathcal{O}(t^8) \quad (14)
\]

\[
N_2 = \frac{L}{2} - 2LT^2 + 7LT^4 + \mathcal{O}(t^6) \quad (13) \quad N_4 = L \frac{t^2}{2} - 2LT^4 + \mathcal{O}(t^6) \quad (15)
\]

This particular case of the generalized \( t-V \) model can be mapped to the Heisenberg XXZ spin model with background magnetic field, which is solved analytically by Orbach [10] and Walker [11]. On closer inspection we can see that the analytical expansions of ground state energy and density-density correlator \( N_1 \) (in the language of spins this is the spin-spin correlator) presented in [11] match our results.

Furthermore, the XXZ model for \( \frac{L}{2} \rightarrow 0 \) is equivalent to the Ising model [12] for which the long-range density-density correlators are:

\[
N_m = \begin{cases} 
0 & \text{for } m \text{ odd} \\
\frac{L}{2} & \text{for } m \text{ even}
\end{cases}
\]

which is fully consistent with our results.

The current density is given by:

\[
J = -it \left\langle \sum_{i=1}^{L} \hat{c}_i^\dagger \hat{c}_{i+1} - \text{h.c.} \right\rangle
\]

and was found to be zero up to order \( \mathcal{O}(t^8) \) for large systems.

Model for \( p = 1 \) was inspected thoroughly in the first order approximation in Refs. [2, 13] where the ground state energy and the current density should both vanish for the half-filling case, which also agrees with our results.
4.2. \( Q = 1/3, p = 2 \) (non-integrable), SCE step 3
For \( p > 1 \) the model is non-integrable. In step 3 (7th order of perturbation), the Hamiltonian is of dimension 36 \( \times \) 36, however it can be divided into three equivalent subspaces of dimension 12 \( \times \) 12. The ground state is therefore 3-fold degenerate and its energy was found to be:
\[
E_0 = -\frac{2L}{3U_2}t^2 + \left( \frac{2L}{3U_2} - \frac{2L}{U_1U_2} \right) t^4 + \left( \frac{16L}{3U_1U_2^3} - \frac{17L}{3U_1^2U_2^2} - \frac{10L}{3U_1^3U_2} \right) t^6 + \mathcal{O}(t^8)
\]
(19)
The density-density correlators are:
\[
N_1 = \frac{2L}{U_1U_2^2} t^4 + \left( \frac{10L}{U_1^2U_2^3} - \frac{34L}{3U_1^3U_2^2} - \frac{16L}{3U_1U_2^3} \right) t^6 + \mathcal{O}(t^8)
\]
(20)
\[
N_2 = \frac{2L}{3U_2^2} t^2 + \left( \frac{4L}{U_1U_2^4} - \frac{2L}{U_1U_2} \right) t^4 + \left( \frac{20L}{3U_1^2U_2^3} + \frac{17L}{U_1U_2^3} - \frac{64L}{3U_1^3U_2^2} \right) t^6 + \mathcal{O}(t^8)
\]
(21)
\[
N_3 = \frac{L}{3} - \frac{4L}{3U_2^2} t^2 + \left( -\frac{16L}{3U_1U_2^4} - \frac{8L}{U_1U_2^3} + \frac{13L}{3U_1^2U_2^2} \right) t^4 + \mathcal{O}(t^6)
\]
(22)
\[
N_4 = \frac{2L}{3U_2^2} t^2 + \left( \frac{10L}{3U_1U_2^3} + \frac{4L}{U_1U_2^2} - \frac{7L}{3U_2^2} \right) t^4 + \mathcal{O}(t^6)
\]
(23)
\[
N_5 = \frac{2L}{3U_2^2} t^2 + \left( \frac{10L}{3U_1U_2^3} + \frac{4L}{U_1U_2^2} - \frac{L}{3U_2^2} \right) t^4 + \mathcal{O}(t^6)
\]
(24)
Similarly to equation (17), we expect that for \( Q = \frac{1}{p+1} \) the density-density correlation functions in the limit of \( \frac{1}{U_m} \to 0 \) to be:
\[
N_m = \begin{cases} 
\frac{L}{p} & \text{for } m \text{ divisible by } p \\
0 & \text{otherwise}
\end{cases}
\]
(25)
and it is indeed true for our results.

Again, the current density is zero up to order \( \mathcal{O}(t^8) \) for large systems.

4.3. \( Q = 1/4, p = 3 \) (non-integrable), SCE step 3
This is another non-integrable case. The Hamiltonian is of dimension 52 \( \times \) 52, but it consists of four equal subspaces of dimension 13 \( \times \) 13. The ground state is thus 4-fold degenerate and has energy:
\[
E_0 = -\frac{L}{2U_3}t^2 + \left( \frac{L}{2U_3} - \frac{3L}{2U_3U_2} \right) t^4 + \left( \frac{4L}{U_3U_2^3} - \frac{17L}{4U_3^2U_2^2} - \frac{5L}{2U_3^2U_2} - \frac{5L}{U_3U_2^3U_3} \right) t^6 + \mathcal{O}(t^8)
\]
(26)
The density-density correlation functions are:
\[
N_1 = \frac{5L}{U_3U_2U_3^2} t^6 + \mathcal{O}(t^8)
\]
(27)
\[
N_2 = \frac{3L}{2U_3^2} t^4 + L \left( \frac{15}{2U_3U_2^3} + \frac{17}{4U_3^2U_2^2} - \frac{4}{U_3U_2^3} + \frac{10}{U_1U_2U_3^2} \right) t^6 + \mathcal{O}(t^8)
\]
(28)
\[
N_3 = \frac{L}{2U_3^2} t^4 - L \left( \frac{3}{2U_3^2} - \frac{3}{U_3U_2^2} \right) t^6 + L \left( \frac{5}{U_3U_2^3} + \frac{51}{4U_3^2U_2^2} - \frac{16}{U_3U_2^3} + \frac{10}{U_1U_2U_3^2} \right) t^6 + \mathcal{O}(t^8)
\]
(29)
\[
N_4 = \frac{L}{4} - \frac{L}{2U_3^2} t^4 + L \left( \frac{13}{4U_3^2} - \frac{4}{U_3U_2^3} - \frac{6}{U_3U_2^3} \right) t^6 + \mathcal{O}(t^8)
\]
(30)
\[
N_5 = \frac{L}{2U_3^2} t^4 + L \left( \frac{2}{U_3U_2^3} + \frac{3}{U_3U_2^3} - \frac{2}{U_3U_2^3} \right) t^6 + \mathcal{O}(t^8)
\]
(31)
Again, our results for correlators are consistent with equation (25).

For a large system size the current density was calculated to be zero up to perturbation order \( \mathcal{O}(t^8) \).
5. Summary & outlook

We have shown that the strong coupling expansion devised for numerically solving lattice quantum field theory problems can also be used in the field of quantum spin models, giving us analytical results. Our test model was the long-range $t$-$V$ model at critical densities. For the integrable system (XXZ model) our results are fully consistent with previous work and for the non-integrable models we have obtained various observables not obtained before.

The next step will be to expand this method to near-critical densities, where there is one additional hole in the system, two additional holes, etc. Though the initial subspace will probably be too big to use analytics, it should be small enough to use numerical approach. The preliminary results show that for a system $p = 2$ (non-integrable), $L = 3N + 1$ (one hole), the Hamiltonian has dimension $2L \times 2L$ in the SCE step 2 and the ground state energy is:

$$E_0 = \begin{cases} \frac{-2t - 2Nt^2 + \frac{2}{U_2} t^3 + \mathcal{O}(t^4)}{L^2} & \text{for odd } N \\ \frac{-2t \cos \frac{\pi}{L} - A(L) \frac{2N}{U_2} t^2 + B(L) \frac{2}{U_2} t^3 + \mathcal{O}(t^4)}{L^2} & \text{for even } N \end{cases}$$

with functions $A(L)$ and $B(L)$ that can be numerically approximated as $A(L) = 1 - \frac{64L(4)}{L^2}$ and $B(L) = 1 + \frac{68L(1)}{L^2} + \frac{1200L(1)}{L^4}$. Further investigation is needed.

The assumption $U_m \lesssim U_m + 1 + U_{m+1}$ that was introduced in the beginning could be also abandoned. The system will now have different phases, depending on the potential energies $U_m$. However, SCE approach should still work if the initial subspace of states is properly chosen for the specific system setup.

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