Spinless fermion model on diamond chain

Onofre Rojas* and S. M. de Souza

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Departamento de Ciencias Exatas, Universidade Federal de Lavras, CP 3037, 37200000, MG, Brazil.

Abstract

The decoration or iteration transformation was widely applied to solve exactly the magnetic spin models in one-dimensional and two-dimensional lattice. The motif of this letter is to extend the decoration transformation approach for models that describe interacting electron systems instead of spin magnetic systems, one illustrative model to be studied, will be the spinless fermion model on diamond chain. Using the decoration transformation, we are able to solve this model exactly. The phase diagram of this model was explored at zero temperature as well as the thermodynamics properties of the model for any particle density. The particular case when particle-hole symmetry is satisfied was also discussed.

Keywords: decoration transformation, spinless fermion, exactly solvable models.

1 Introduction

Exactly solvable models in statistical physics and mathematical physics is one of the most challenging topics. Recently several exactly solvable models were studied in quasi-one dimensional classical-quantum models such as Ising-Heisenberg models[1, 2, 3, 4, 5, 6], as well as two-dimensional Ising models and Ising-Heisenberg models[7, 8], that can be mapped onto exactly solvable vertex models. Although the decoration transformation was introduced in the fifty decade[9, 10], in order to study the decorated spin models. Due to a successful application of this approach, recently this method was extended for a general case of decoration transformation[11], later extended by Strecka[12] even for classical-quantum models such as Ising-Heisenberg models. Recently another interesting application of decoration transformation was also investigated by Pereira et al.[13] where they considered a delocalized interstitial electrons on diamond-like chain and they also investigate the magnetocaloric effect in kinetically frustrated diamond chain[14], meanwhile Strecka et al.[15] discussed the localized Ising spins and itinerant electrons in two-dimensional models, as well as two-dimensional spin-electron with coulomb repulsion[16].

On the other hand studies of strongly correlated electron systems are certainly one of the most important areas of condensed matter physics. A large number of papers have been concerned with the investigation of heavy-fermion behavior, magnetism of strongly correlated systems, high temperature superconductivity, or metal–insulator transitions and charge-ordering phenomena. A limiting case of these systems could be the spinless fermion model, where the spin orientation could be ignored or it can be understand as a fully polarized system. The one-dimensional case of this model already was investigated by Czart[17] and Zhuravlev et al.[19]. Although spinless fermion models can be transformed onto XXZ models in a magnetic field parallel to the anisotropy[17, 19] by the use of the well known Jordan-Wigner transformation, this kind of mapping could be more involving for the Hubbard-like systems, where the spin orientation is considered. Therefore, the purpose here is how to use the decoration transformation approach for interacting electron systems, without mapping onto spin models.

The outline of this letter is as follow: In sec. 2 we introduce the model to be studied. In sec. 3 we present the phase diagram at zero temperature. In sec. 4 is devoted the decoration transformation and transfer matrix approach, in order to obtain its exact solution. Whereas in sec. 5 is discussed the thermodynamics, particle density and correlation function of the model considered, and finally in sec. 6 we present our conclusions.

*email: ors@dex.ufla.br; phone: +5535 38291954; fax: +5535 38291961.
where $a_{\alpha,i}(a_{\alpha,i}^\dagger)$ are Fermi annihilation (creation) operators for spinless (or completely polarized) fermion respectively, with $\alpha = \{a, b, c\}$, while $n_{\alpha,i} = a_{\alpha,i}^\dagger a_{\alpha,i}$ being number operators. The Hamiltonian parameter $t$ is the hopping term (solid lines), $\mu$ is the chemical potential, and the Coulomb repulsion term between fermions on neighboring sites (dashed lines) is represented $V$ and $V_1$. We also consider a periodic boundary condition.

The spinless fermion model on diamond chain, has an important particle–hole symmetry[18]. For the purpose of this discussion, the following canonical transformation $a_{\alpha,i}^\dagger \rightarrow a_{\alpha,i}$ and $a_{\alpha,i} \rightarrow a_{\alpha,i}^\dagger$ was considered. For the occupation number operator the transformation reads $n_{\alpha,i} \rightarrow a_{\alpha,i}a_{\alpha,i}^\dagger = 1 - n_{\alpha,i}$, thus the transformed Hamiltonian becomes

$$H_{i,i+1} = -t \left(a_{a,i}^\dagger a_{b,i} + a_{b,i}^\dagger a_{a,i}\right) - \mu \left(n_{a,i} + n_{b,i} + \frac{1}{2}(n_{c,i} + n_{c,i+1})\right)$$

$$+ V_1 n_{a,i} n_{b,i} + V_2 \left(n_{c,i} + n_{c,i+1}\right)\left(n_{a,i} + n_{b,i}\right),$$

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$$H'_{i,i+1} = t \left(a_{a,i}^\dagger a_{b,i} + a_{b,i}^\dagger a_{a,i}\right) - (V + V_1 - \mu)(n_{a,i} + n_{b,i}) - (V - \mu/2)(n_{c,i} + n_{c,i+1})$$

$$+ V_1 n_{a,i} n_{b,i} + V_2 \left(n_{c,i} + n_{c,i+1}\right)\left(n_{a,i} + n_{b,i}\right) + (V_1 + 2V - 3\mu).$$

The different signs of the hopping term on sites $a$ and $b$ can be compensated by a further canonical transformation as follows. By formally replacing say $a_{a,i}^\dagger \rightarrow -a_{a,i}^\dagger$ ($a_{a,i} \rightarrow -a_{a,i}$) for $a$ sites, but keeping unchanged the operators on sites $b$, or vice-versa.

On the other hand, using the Jordan-Wigner transformation it is possible to map the spinless fermion diamond chain onto a Ising-Heisenberg diamond chain with non-uniform external magnetic field, as discussed in reference[15], the $z$-component of the spin-1/2 operator is related to number operator by $n = \sigma^z + 1/2$, while the creation (annihilation) operators are related through $a_{j}^\dagger = 2\left(\prod_{k<j} \sigma_k^z\right) \sigma_j^+$ and $a_j = 2\left(\prod_{k<j} \sigma_k^z\right) \sigma_j^-$. Therefore the models are related through the relations $J_H = V_1$, $J_I = V$, $H_H = \mu - (V + V_1)/2$, $H_I = \mu - V$ and $J_H \Delta = -t/2$.

The Hamiltonian of spinless fermion model on diamond chain, has not been discussed yet anywhere. In this sense discussing this model, we could be opening several variants of fermion models and the most interesting models are the extended Hubbard-like models[20] with decorated interactions, where is taking into account the spin orientation, that is why it is interesting first to discuss the spinless fermion model.
3 The phase diagram

Considering the state vectors, where hopping term \( t \) is acting at sites \( a \) and \( b \). In each state there are only two possibilities labeled by 0 or 1, it means an empty or occupied particle state respectively, this leads to the following state vector \( |\Psi\rangle = c_1|0,0\rangle + c_2|0,1\rangle + c_3|1,0\rangle + c_4|1,1\rangle \), where \( c_i \) are the coefficients to be determined for each state.

The states acting on Hamiltonian \( \mathbf{H} \) at sites \( a \) and \( b \) for each elementary cell becomes,

\[
H_{i,i+1}|0,0\rangle = -\frac{\mu}{2}(n_{c,i} + n_{c,i+1})|0,0\rangle, \quad (4)
\]

\[
H_{i,i+1}|0,1\rangle = \left[ \left( \frac{V}{2} - \frac{\mu}{2} \right) (n_{c,i} + n_{c,i+1}) - \mu \right]|0,1\rangle - t|1,0\rangle, \quad (5)
\]

\[
H_{i,i+1}|1,0\rangle = \left[ \left( \frac{V}{2} - \frac{\mu}{2} \right) (n_{c,i} + n_{c,i+1}) - \mu \right]|1,0\rangle - t|0,1\rangle, \quad (6)
\]

\[
H_{i,i+1}|1,1\rangle = \left[ \left( V - \frac{\mu}{2} \right) (n_{c,i} + n_{c,i+1}) + V_1 - 2\mu \right]|1,1\rangle. \quad (7)
\]

After diagonalize the above \( 4 \times 4 \) matrix we have 4 eigenvalues, these eigenvalues depends only on the number of operators \( n_{c,j} \), along with the Hamiltonian parameters. The states \( (4) \) and \( (7) \) are already in their eigenstates, while the eigenvalues of eqs. \( (5) \) and \( (6) \) is given simply by \( \left[ \left( \frac{V}{2} - \frac{\mu}{2} \right) (n_{c,i} + n_{c,i+1}) - \mu \right] \pm t \), whereas their respective eigenvectors are given by \( |\psi\rangle_{s,a} = \frac{1}{\sqrt{2}}(|0,1\rangle \pm |1,0\rangle) \), symmetric and anti-symmetric states respectively. Although there are 16 eigenvalues only four possible ground states energies were found, whose eigenvectors for different phases are given by

\[
|S0\rangle = \prod_{i=1}^{N} (|0,0\rangle_i \otimes |0\rangle_i), \quad \rho = 0, \quad (8)
\]

\[
|S1\rangle = \prod_{i=1}^{N} \frac{1}{\sqrt{2}} (|1,0\rangle_i + |0,1\rangle_i) \otimes |0\rangle_i, \quad \rho = 1, \quad (9)
\]

\[
|S2\rangle = \prod_{i=1}^{N} \frac{1}{\sqrt{2}} (|1,0\rangle_i + |0,1\rangle_i) \otimes |1\rangle_i, \quad \rho = 2, \quad (10)
\]

\[
|S3\rangle = \prod_{i=1}^{N} (|1,1\rangle_i \otimes |1\rangle_i), \quad \rho = 3, \quad (11)
\]

where the states of type \( |a,b\rangle \otimes |c\rangle \) corresponds to the particles states at sites \( a, b \) and \( c \), respectively.

The ground state phase diagram of \( V \) as a function of \( \mu \) is displayed in fig. \[2\] for fixed values of \( t = 1 \) and \( V_1 = V \). The four states are limited as follow:

\[|S0\rangle : \text{limited by } \mu \leq -1, \text{ with } \rho = 0, \quad (12)\]

\[|S1\rangle : \text{between } \mu \geq -1 \text{ and } V = \mu \text{ with } \rho = 1, \quad (13)\]

\[|S2\rangle : \text{between } V = \mu \text{ and } V = (\mu - 1)/2 \text{ with } \rho = 2, \quad (14)\]

\[|S3\rangle : \text{between } V = (\mu - 1)/2 \text{ and } V = 0 \text{ with } \rho = 3. \quad (15)\]

The first one is |\( S0 \rangle \), this corresponds just to a simple empty lattice particle (or fully-filled holes) on diamond chain with total density \( \rho = 0 \) (yellow region). The second state is represented by |\( S1 \rangle \), where one particle is at site \( a \) or \( b \) of the elementary cell, then the particle density for this state is \( \rho = 1 \) (green region). Furthermore
there is another state $|S_2\rangle$, this state corresponds to the configuration that one particle is fluctuating at sites $a$ and $b$, whereas on site $c$ of elementary cell there is another particle, then the total density is $\rho = 2$ (red region). Finally there is a fully-filled particle diamond chain state represented by $|S_3\rangle$ with density $\rho = 3$, or it can also be understood as an empty lattice of hole state (blue region).

### 4 Decoration transformation and transfer matrix

In order to study the thermodynamics properties of the spinless fermion model on diamond chain, it will be used the decoration transformation \cite{10, 11, 12} as described below. Actually, it is not necessary to map the spinless fermion model onto spin models, like Ising-Heisenberg model \cite{1, 2, 3, 4, 6}. Thus, there is an interest in performing the decoration transformation for operators. In this sense it will be apply directly the decoration transformation approach \cite{10, 11, 12} for the proposed model. The main aim to solve the Hamiltonian (1) of spinless fermion model on diamond chain is to map onto an effective spinless fermion model without hopping term, whose Hamiltonian is given by

\begin{equation}
\tilde{H} = \sum_{i=1}^{N} \left[ \tilde{V} n_{c,i} n_{c,i+1} - \frac{\tilde{\mu}}{2} (n_{c,i} + n_{c,i+1}) \right],
\end{equation}

where $\tilde{V}$ and $\tilde{\mu}$ are coefficients to be determined using decoration transformation \cite{10, 11}.

The Boltzmann factor of effective spinless fermion model can be expressed as follow

\begin{equation}
\tilde{w}(n_{c,i}, n_{c,i+1}) = \exp \left( \beta \tilde{V} n_{c,i} n_{c,i+1} - \beta \frac{\tilde{\mu}}{2} (n_{c,i} + n_{c,i+1}) \right),
\end{equation}

where $\beta = 1/kT$, with $k$ being the Boltzmann constant and $T$ the absolute temperature.

On the other hand the Boltzmann factors for the spinless fermion model on diamond chain given for the Hamiltonian (1) reads as
\[ w(n_{c,i}, n_{c,i+1}) = \text{tr}_{a,b} \left( e^{-\beta H_{c,i+1}} \right), \]

the operators \( n_{c,i} \) ranges from 0 to 1, then we have explicitly the Boltzmann factors,

\[
\begin{align*}
    w(0,0) &= 1 + 2e^{\beta \mu} \cosh(\beta t) + e^{-2V_1 + 2\beta \mu}, \\
    w(0,1) &= e^{\beta \mu/2} + 2e^{\beta \mu/2 - \beta V/2} \cosh(\beta t) + e^{-\beta (V + V_1) + 5\beta \mu/2}, \\
    w(1,1) &= e^{\beta \mu} + 2e^{\beta \mu - \beta V} \cosh(\beta t) + e^{-\beta (2V + V_1) + 5\beta \mu}. 
\end{align*}
\]

For simplicity the Boltzmann factor for diamond chain are denoted by \( w_0 = w(0,0) \), \( w_1 = w(1,0) = w(0,1) \) and \( w_2 = w(1,1) \).

In order to apply decoration transformation we need to impose the following condition:

\[ Z = f Z_{\text{eff}}. \]  

The Boltzmann factor for both systems must be equal in order to satisfy the decoration transformation\[^{10, 11}\].

Thus there are three unknown algebraic equations and three unknown parameters, this algebraic system is solved easily using the decoration transformation method, whose solutions are written as

\[
\begin{align*}
    f &= w_0, \quad \tilde{\mu} = \frac{2}{\beta} \ln \left( \frac{w_1}{w_0} \right), \quad \tilde{V} = \frac{1}{\beta} \ln \left( \frac{w_2^2}{w_1^2 w_0} \right)
\end{align*}
\]

where the \( f, \tilde{\mu} \) and \( \tilde{V} \) are expressed as a functions of the original parameters of the Hamiltonian by means of \( w_0, w_1 \) and \( w_2 \).

On the other hand, the Boltzmann factor for effective spinless fermion model reads as

\[
\begin{align*}
    \tilde{w}_0 &= 1, \quad \tilde{w}_1 = e^{\beta \tilde{\mu}/2} = x, \quad \tilde{w}_2 = e^{\beta \tilde{\mu} - \beta \tilde{V}} = x^2 y,
\end{align*}
\]

with being \( x = \exp(\beta \tilde{\mu}/2) \) and \( y = \exp(-\beta \tilde{V}) \).

In what follows, we are interested to solve the effective spinless fermion without hoping term (also known as the atomic limit), to solve this effective model it will be used the transfer matrix method\[^{21}\], given by

\[ T = \begin{pmatrix} 1 & x & x^2 \\ x & y & x^2 y \end{pmatrix}. \]

Note that the terms \( \tilde{\mu} \) and \( \tilde{V} \) can be obtained in a similar way as were obtained for spin models. The eigenvalues of transfer matrix are given by \( \lambda_\pm = \left( 1 + yx^2 \pm \sqrt{(1 - yx^2)^2 + 4x^2} \right)/2. \)

Using the largest eigenvalues \( \lambda_+ \) of the transfer matrix \( T \), we obtain the partition function per site of the model in terms of the effective spinless fermion model in atomic limit \( Z = f Z_{\text{eff}} \), with \( Z_{\text{eff}} = \lambda_+ \) is the partition function for effective spinless fermion without hopping term. The partition function per elementary cell, is expressed in terms of the Boltzmann factors for the spinless fermion model on diamond chain, may be written

\[ Z = \frac{1}{2} \left( w_0 + w_2 + \sqrt{(w_0 - w_2)^2 + 4w_2^2} \right). \]

From the partition function of spinless fermion model on diamond chain, it is possible to obtain the free energy by the relation \( \Omega = -kT \ln Z \). Once known this result, we are ready to study several physical amounts such as entropy, specific heat, average energy and so on.
\[ V = 1 \quad \text{and} \quad V_1 = 1 \]

\[ V = 1 \quad \text{and} \quad V_1 = 0 \]

\[ V = 1 \quad \text{and} \quad V_1 = 0 \]

\[ V = 1 \quad \text{and} \quad V_1 = 0 \]

\[ (a) \ V = 1 \quad \text{and} \quad V_1 = 1 \]

\[ (b) \ V = 1 \quad \text{and} \quad V_1 = 0.1 \]

\[ (c) \ V = 1 \quad \text{and} \quad V_1 = 1 \]

\[ (d) \ V = 1 \quad \text{and} \quad V_1 = 0.1 \]

Figure 3: In (a) and (b) is plotted the total density \( \rho \) as a function of chemical potential \( \mu \), for fixed values of temperature. In (c) and (d) we display the amount \( \langle n_a \rangle - \langle n_c \rangle \) versus \( \mu \), for same set of parameters.

5 Thermodynamics and correlation functions

So far, we have not yet specified the particles number of the diamond chain. In order to obtain the electron density per elementary cell, we take the derivative of free energy in relation to the chemical potential of spinless fermion on diamond chain

\[ \rho = -\frac{\partial \Omega}{\partial \mu} \bigg|_\beta = 2 \langle n_a \rangle + \langle n_c \rangle, \quad (27) \]

here we are assuming the exchange invariance of sites \( a \) and \( b \).

The particle density of type \( c \) can be obtained from effective spinless fermion model, by the relation

\[ \langle n_c \rangle = \frac{1}{1 + \left( \lambda^2 + 1 \right)^2}, \quad (28) \]

whereas the particle density for sites \( a \) and \( b \) per site, can be obtained combining eqs. (27) and (28), resulting in

\[ \langle n_a \rangle = \rho - \langle n_c \rangle. \quad (29) \]

Further we illustrate the chemical potential behavior for fixed values of \( t = 1, V = 1 \) and \( V_1 = \{1, 0.1\} \). In fig. 3(a-b) we display the density \( \rho \) as a function of chemical potential \( \mu \), for a range of temperatures \( T = 1.0, 0.4, 0.1 \) and 0.01, this behavior is in agreement with phase transition at zero temperature (fig. 2) discussed previously. We show three plateaus at low temperature, when \( \rho \) becomes 1, 2 or 3. The size of plateau at density \( \rho = 2 \) is proportional the parameter \( V_1 \), for small \( V_1 \) there is a short plateau (fig. 3(b)), while for large \( V_1 \) long plateau is observed (the last one not illustrated). In fig. 3(c-d) the amount \( \langle n_a \rangle - \langle n_c \rangle \) versus \( \mu \) is displayed, in order to study the average particles number behavior at sites \( a \) and \( b \) compared to that one on site \( c \). So for negative chemical potential we have \( \langle n_a \rangle > \langle n_c \rangle \), while for positive chemical potential we have \( \langle n_a \rangle < \langle n_c \rangle \).

Another interesting properties we would like to discuss is the symmetry particle-hole described by eqs (3) must be satisfied only when \( V_1 = V \), therefore we find the following relation for the free energy,

\[ \Omega(t, V, \mu) = \Omega(t, V, 2V - \mu) + (3V - 3\mu). \quad (30) \]

In general, the chemical potential depends on the temperature, however at half-filled band particle density \( \rho = 1.5 \) and under particle-hole symmetry relation, the chemical potential becomes independent of the temperature, given simply by \( \mu = V \). If we look at the phase diagram displayed in fig. 2, the relation \( V = \mu \) corresponds the phase transition between density \( \rho = 1 \) and 2, as expected the density in this region should be \( \rho = 1.5 \), due to the thermal fluctuation begins to act.
Furthermore, in fig. 4 the chemical potential as a function of the temperature for fixed values of density $\rho$ is displayed; from this plot we may conclude that there is a chemical potential independent on the temperature only at half-filled band and when symmetry particle-hole is satisfied.

Another interesting quantity we would like to comment is the correlation function, it can also be obtained using transfer matrix method[21], which after some algebraic manipulation we obtain,

$$\langle n_{c,r}n_{c,r+k}\rangle = \langle n_c\rangle^2 + \frac{\langle n_c\rangle}{1 + \left(\frac{\lambda}{\lambda^+}\right)^2} \left(\frac{\lambda}{\lambda^+}\right)^k. \tag{31}$$

Some other nearest correlation or expected values of higher order can be obtained, combining the derivative of diamond chain Hamiltonian with respect to one of its parameter, and the decoration transformation for correlation function as discussed in reference [10, 11].

### 6 Conclusions

Although the decoration transformation has originally been developed to study magnetic spin models[10,11,12], and since then, this method was widely applied to solve several decorated spin models. Motivated by this successful application, this transformation later was generalized[11], and recently Strecka[12] extended even for Ising-Heisenberg spin models. However, there is no any approach developed for electron interacting systems, such as strongly correlated electron systems. In this sense, we discuss how the decoration transformation can also be used to map from one decorated electron system onto another effective electron system. As an illustrative application of decoration transformation for electron interacting models, it has been considered the spinless fermion model on diamond chain, where vertical solid line corresponds to hopping term and repulsive Coulomb interaction term, while by dashed line we mean the repulsive Coulomb interaction term between the nearest neighbor (fig. 1). Furthermore, we discuss some properties of this model, such as the phase diagram at zero temperature, showing four different states with a given number of particles, changing from empty lattice (or fully-filled holes) of particles to fully-filled particles (or empty lattice of holes) on the diamond chain. The thermodynamics of this model, allows to display the particle density as a function of chemical potential per elementary cell as well as the chemical potential as a function of temperature. Finally an additional quantity also was considered such as the correlation function.
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