An Orthofermion Approach for Thermodynamic Properties of Infinite U Hubbard Model in one and two Dimensions

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Abstract. Hubbard model plays a critical role in the study of strongly correlated electron systems. The only available exact solutions of 1-D Hubbard Hamiltonian, obtained through nested Bethe ansatz, show a spin charge decoupling for infinite $U$ when there is no possibility of double occupancy of an electron orbital state. It had been shown that these features can be directly obtained by employing orthofermion algebra. In the present communication, the thermodynamic properties, namely, specific heat and entropy are provided for a 1-D chain and 2-D square lattice using orthofermion approach. It is shown that in 1-D, our results are identical to the known exact results. We have also compared the thermodynamic properties of free fermions and orthofermions in both 1-D and 2-D. Our thermodynamic results, based on orthofermion approach, can be used to ascertain the accuracy of the approximate methods employed in the context of infinite $U$ Hubbard model.

1. Introduction

The Hubbard model provides the simplest Hamiltonian describing a correlated electron system [1]. The $U$ infinity limit of the Hubbard Hamiltonian has come to occupy a central role in the context of strongly correlated electron systems. It has been extensively employed in the context of high temperature superconductivity as well as for understanding the magnetic properties of correlated systems, as described by $t - J$ Hamiltonian. An important consequence of infinite intrasite electron repulsion $U$ is that each electron orbital state can be utmost occupied by a single electron, irrespective of its spin direction.

Obtaining solutions of Hubbard Hamiltonian remains a challenging task. Till date, only exact solution of the Hubbard Hamiltonian is available for a 1-D system through the application of nested Bethe ansatz ($NBA$) approach [2]. Even in one dimension, although we have a fairly complete description of the ground state properties by the exact $NBA$ solutions, there exist very few exact results at finite temperatures. Exact analytical expressions for the thermodynamic properties for $U = \infty$ have been derived by many authors in one dimension, but their methods cannot be extended to higher dimensions[3, 4, 5, 6]. However, it has been shown that orthofermion approach not only reproduces the known exact 1-D results for infinite $U$, but can also be used to obtain 2-D results [7].
In the present communication, we obtain the thermodynamic properties of noninteracting orthofermions in one and two dimensions, and compare the results with non interacting fermions having identical particle density.

2. Orthofermion algebra and nested Bethe ansatz solutions
Nested Bethe ansatz solutions exhibit nontrivial consequences in the $U\infty$ limit. As highlighted by Fulde, a remarkable property of the $U\infty$ NBA wavefunctions is that their spatial part correspond to that of spin-less fermions for any distribution of particles or holes on the chain [8, 9, 10]. This general feature of the NBA state vectors automatically implements the ‘no double-occupancy’ constraint. Unlike in the Gutzwiller projection operator approach (GPO), no additional projection operators are required. It is pertinent to point out that in the presence of holes, the NBA wave function is a superposition of spin-charge factorized wavefunctions. It may be noted that in contrast to orthofermion approach, GPO fails to reproduce the the exact energy spectrum in the $U\infty$ limit [11].

The orthofermion algebra automatically satisfies the requirement of no double occupancy and spin charge decoupling as exhibited by the NBA solutions. It also extends the exact 1-D solutions of infinite $U$ Hubbard model to the higher dimensions in a very simple and natural way.

3. Thermodynamic Properties
The Hamiltonian for a system of noninteracting orthofermions, in wave vector space, is given as

$$H = \sum_{k\sigma} (\epsilon_k - \mu) a_{k\sigma}^\dagger a_{k\sigma}$$

where orthofermion creation and annihilation operators satisfy the algebra

$$a_{k\alpha}^\dagger a_{k'\beta}^\dagger + a_{k'\alpha}^\dagger a_{k\beta}^\dagger = \delta_{kk'}\delta_{\alpha\beta}; \quad a_{k\alpha} a_{k'\beta}^\dagger = \delta_{\alpha\beta}(\delta_{kk'} - \sum_{\gamma} a_{k'\gamma}^\dagger a_{k\gamma})$$

The various thermodynamic quantities can be obtained using the the orthofermion partition function

$$Z_{of} = \prod_k (1 + e^{-\beta(\epsilon_k - \bar{\mu})})$$

where

$$\bar{\mu} = \mu + \frac{1}{\beta} \ln(2)$$

Since the thermal average of any operator $O$ is given by $<O> = Tr(Oe^{-\beta H})/Z$, the distribution function $<n_k> = \sum_{\sigma} a_{k\sigma}^\dagger a_{k\sigma}$ is given as

$$<n_k> = -\frac{1}{\beta} \frac{\partial \ln Z}{\partial \epsilon_k} = \frac{1}{e^{\beta(\epsilon_k - \bar{\mu})} + 1}.$$  

The above distribution function has been obtained earlier by Kwak and Beni [5] for the infinite $U$ Hubbard model in absence of magnetic field.

Using the partition function (3), we get entropy $S$ and the specific heat $C_v$ as

$$S = -k \sum_k [<n_k> \ln <n_k> + (1 - <n_k>) \ln(1 - <n_k>)] + Nk \ln(2)$$

$$C_v = k\beta^2 \sum_k \epsilon_k^2 <n_k> (1 - <n_k>) - \frac{(\sum_k \epsilon_k <n_k> (1 - <n_k>))^2}{\sum_k <n_k> (1 - <n_k>)}$$
For a system of free fermions, Hamiltonian has the same form as that of orthofermions, given by eq (1), with orthofermion creation and annihilation operators being replaced by fermion creation and annihilation operator. The thermodynamic expressions (3) to (7) are of the same form except we have to replace $\bar{\mu}$ by $\mu$ and $k$ by $k\sigma$, and omit the second term $Nk \ln(2)$ in the expression of the entropy. In case of orthofermions this term is free spin entropy because of spin charge separation.

Both for fermions and orthofermions, the energy $\epsilon_k$ equals to $2\Delta \cos(k)$ for a 1-D system and $2\Delta(\cos(k_x) + \cos(k_y))$ for a two dimensional square lattice. $\Delta$ is the hopping term. Using these relations we provide the thermodynamic quantities in the next section.

4. Results and Discussions

The results corresponding to the dependence of entropy and specific heat per particle on the temperature for the average particle densities $n = 0.2, 0.5$ and $0.8$, both for orthofermions and fermions, are presented in this section. It may be noted that for a 1-D system, the thermodynamic quantities obtained by orthofermion approach exactly coincide with the results of Klein, obtained through a projected Hubbard Hamiltonian [12]. One draw back of Klein approach is that the creation and annihilation operators introduced therein violate particle and spin number conservation. No such limitation exists for orthofermion creation and annihilation operators. For a better comparison of the results, plots for fermions and orthofermions appear in the same figure.

The results for entropy vrs temperature in 1-D system are plotted in FIG. 1. In contrast to entropy of fermions, which tends to zero as temperature nears zero, the entropy of orthofermions remains finite at zero temperature. For orthofermions statistics, entropy has an additional contribution of $nk \ln(2)$, because of free spins. Therefore at low temperature, entropy of fermions are lower than orthofermions entropy, though for larger temperature this trend gets reversed.

Variation of specific heat with respect to temperature for different particle densities is provided in FIG. 2. The specific heat tends to zero as $T \to 0$ for fermions and orthofermions. The orthofermion specific heat exhibits a particle-hole symmetry and specific heat for a given $n$ and $1-n$ are identical. On the other hand fermion specific heat keeps on increasing for moderate and large temperatures with increasing particle density, though at low temperature, this trend again gets reversed. Consequently, the specific heat tends to zero more steeply with decreasing temperature as the fermion density diminishes. Other important outcome of the calculations is
that for not very low temperatures, specific heat for fermions remains larger than orthofermion specific heat for identical particle densities.

The trends noted in the thermodynamic quantities vs temperature plots for 1-D lattice remains valid for fermions and orthofermions on a 2-D square lattice. The difference between the entropy of both kind of particles in 1-D and 2-D square lattice are not appreciable (FIG. 3). However, the variation in the specific heat at low enough temperature is now smoother (FIG. 4). The specific heat for fermions and orthofermions do not show a crossover behaviour with varying particle density in the low temperature regime for a 2-D square lattice. Also the particle-hole symmetry for orthofermions specific heat for the particle densities considered here remains valid.

5. Summary and Conclusions
Thermodynamic properties of free orthofermions on a 1-D lattice have been determined. The 1-D results coincide with the earlier known exact results in the $U$ infinity limit of Hubbard Hamiltonian. As the earlier methods could not be extended to higher dimensions, orthofermion approach has been used to study the consequences of $U$ infinity limit in 2-D, particularly, for a square lattice. The orthofermion results obtained here have been compared with the thermodynamic properties of noninteracting fermions in 1-D and 2-D. Besides, the similarity and differences between the the thermodynamic properties of orthofermions in 1 and 2-Dimensions have been highlighted.

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