Thermodynamic and transport properties of infinite U Hubbard model

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Abstract. The infinite U Hubbard model, which excludes double occupancy of electrons on a lattice site, can be considered as an exactly solvable non-interacting orthofermion model. We obtained several thermodynamic and transport properties like specific heat, entropy, magnetization, magnetic susceptibility and thermoelectric power for the non-interacting orthofermions. It is found that in one dimension our results coincide with that of known exact results. In case of thermoelectric power, we have also obtained the generalized Heikes formula in high temperature limits and Stafford results at low temperatures. Since the non-interacting orthofermion model is exactly solvable in any dimension, our results can be used as a guide to ascertain the accuracy of the approximations, used to solve the finite U Hubbard model, frequently employed for the study of the strongly correlated electron systems.

1. Introduction

The Hubbard model [1] has been widely used for the theoretical description of electronic states in strongly correlated electron systems. For strongly correlated electron systems with large intra-atomic interaction U of the Hubbard model, there are formidable problems for its solutions in dimensions higher than one. Even in one dimension, although we have a fairly complete description of the ground state properties by the exact nested Bethe ansatz solutions [2], there exist very few exact results at finite temperatures. Exact analytical expressions for thermodynamic and transport properties for $U = \infty$ have been derived by many authors [3, 4, 5, 6] in one dimension. However their methods cannot be extended to higher dimensions.

The orthofermion approach [7] extends the one dimensional solutions of the infinite U Hubbard model to the higher dimensions in a very simple and natural way. For the infinite U, the electrons avoid double occupancy of lattice sites and the Hubbard Hamiltonian is equivalent to the Hamiltonian of noninteracting orthofermions [7]. The algebra of the orthofermion creation and annihilation operators automatically satisfies the requirement of no double occupancy and spin charge decoupling as required by the nested Bethe ansatz solutions for one dimensional infinite U Hubbard model. In addition, it has been shown [8] that for the infinite U, the fermion based Gutzwiller projection operator approach fails to recapture the essential physics and the orthofermion approach is equivalent to the nested Bethe ansatz solutions.

In Sec. 2, we obtain the thermodynamic properties like specific heat, entropy, magnetization, magnetic susceptibility for the non-interacting orthofermions in presence of a magnetic field. We compare our results with the known exact results in one dimension and show the spin charge decoupling in all the thermodynamic properties. In Sec. 3, the thermoelectric power is obtained...
and it is compared with the known exact results in one dimension as well as in low and high temperature limits. Finally in Sec. 4 we give our concluding remarks.

2. Thermodynamic properties

On taking the Fourier transform, the Hamiltonian of the noninteracting orthofermions [9], $H = \sum_{ij \sigma} t_{ij} a_i^{\dagger} a_j \sigma - \mu \sum_{\sigma} n_{\sigma}$, in presence of a constant magnetic field $B$ in the $z$ direction can be written as

$$H = \sum_k H_k \; ; \; H_k = (t_k - \mu)n_k - 2B\mu_B \sum_k S_k^z,$$

(1)

where $t_k$ is the Fourier transform of $t_{ij}$, $\mu_B$ is the Bohr magneton, $S_k^z$ is the $z$ component of the spin operator and $n_k = \sum_{\sigma} n_{k\sigma} = \sum_{\sigma} a_{k\sigma}^{\dagger} a_{k\sigma}$ is the number operator for the state $k$.

The thermodynamic properties can be obtained from the partition function $Z = Tr e^{-\beta H} = \prod_k Tr e^{-\beta H_k}$. Here, $\beta = 1/kT$ is inverse of the product of temperature $T$ and the Boltzmann constant $k$. It has been shown [9] that the eigenvalues of the number operator $n_k$ are either zero or one and the eigenvalues of the spin operator $S_k^z$ are zero for $n_k$ equal to zero and $\pm1/2$ for $n_k$ equal to one. Hence the partition function reduces to,

$$Z = \prod_k (1 + e^{-\beta(t_k - \mu)}), \quad \text{with} \quad \mu = \mu + \frac{1}{\beta} \ln(2 \cosh(\beta B\mu_B))$$

(2)

Eqn. (2) have been obtained earlier for the infinite U Hubbard model in one dimension [10]. Since the thermal average of any operator $O$ is given by $<O> = Tr(Oe^{-\beta H})/Z$, the distribution function $<n_k>$ is given as

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

(3)

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

As the thermodynamic quantities namely energy ($E$), specific heat ($C_v$), entropy ($S$), magnetization ($M$), and the susceptibility ($\chi$) are related to the partition function $Z$ [11], we obtain these as

$$E = \sum_k t_k <n_k> - NB\mu_B \tanh(\beta B\mu_B),$$

(4)

$$C_v = k\beta^2 \left[ \sum_k t_k^2 <n_k> (1-<n_k>) - \frac{\left( \sum_k t_k <n_k> (1-<n_k>) \right)^2}{\sum_k <n_k> (1-<n_k>)} \right] + \frac{Nk(\beta\mu_B)^2}{\cosh^2(\beta\mu_B)}$$

(5)

$$S = k \sum_k [<n_k> \ln<n_k> + (1-<n_k>) \ln(1-<n_k>)] + Nk[\ln(2 \cosh(\beta B\mu_B)) - \beta B\mu_B \tanh(\beta B\mu_B)]$$

(6)

$$M = N\mu_B \tanh(\beta B\mu_B) \quad \text{and} \quad \chi = \frac{N\mu_B^2}{kT}.$$  

(7)

Eqns. (4) (5) and (6) reduce to the exact one dimensional results of Klein [3], obtained for the infinite U Hubbard model in absence of magnetic field. In these expressions, first term corresponds to the contribution due to spinless fermions and the second term represents the contribution due to free spins in a magnetic field. Thus these results show that there is spin charge decoupling in all dimensions. In Eqn. (7) both magnetization and susceptibility correspond to free spins values as shown by Sokoloff [4] in one dimension for the infinite U Hubbard model.
3. Thermoelectric Power

The thermoelectric power of strongly correlated electron systems have received a lot of attention after the observation of a very large room temperature thermoelectric power in the strongly correlated material, NaCo$_2$O$_4$ [12]. Measurements of the thermoelectric power in metallic organic material [13, 14] have also been found to be describable by models of strongly interacting electrons on a lattice, like Hubbard model.

In order to calculate the thermoelectric power, we shall use the Kubo formalism [15] of the transport coefficients of a many body system. In this formalism, the thermoelectric power ($S_T$) can be expressed as

$$S_T = 1 \frac{1}{eT} \int_0^\infty dt \int_0^\infty d\lambda <Q_x(-i\hbar \lambda)v_x(t)> - \mu).$$

(8)

For the sake of convenience, but without any loss of generality, we have considered the transport in the x direction, perpendicular to the magnetic field B, applied in the z direction. $v_x(t)$ and $Q_x(t)$ are the velocity and the energy flux operators in the Heisenberg representation along the x direction, V is the volume of the system, and e is electron charge. The velocity and the energy flux operators v and Q can be easily obtained from the continuity equations. It is found that they commute with the Hamiltonian (1) and therefore are independent of time. In this case the first term on the right hand side of the above equation reduces to a simple form $<Q_xv_x>$. The correlation functions $<Q_xv_x>$ and $<v_x^2>$ are given as

$$<Q_xv_x> = \frac{1}{h^2} \sum_{k_1,k_2 \sigma} (t_{k_1} - \sigma B \mu B) \Delta_{k_1} t_{k_1} \Delta_{k_2} t_{k_2} <n_{k_1 \sigma} n_{k_2}>$$

(9)

$$<v_x^2> = \frac{1}{h^2} \sum_{k_1,k_2} \Delta_{k_1} t_{k_1} \Delta_{k_2} t_{k_2} <n_{k_1} n_{k_2}>$$

(10)

The two particle correlation functions $<n_{k_1} n_{k_2}>$ and $<n_{k_1 \sigma} n_{k_2} \sigma>$, which appear in Eqns. (9) and (10), can be obtained from one and two particle Green’s functions, $G_{k \sigma}(\omega) = <=a_{k \sigma}^\dagger a_{k \sigma}>_\omega$ and $G_{k_1 k_2}(\omega) = <=a_{k_1 \sigma_1}^\dagger a_{k_2 \sigma_2}^\dagger a_{k_2 \sigma_2} a_{k_1 \sigma_1}>_\omega$ (for notations see Zubarev [16]). For the system of noninteracting orthofermions, described by the Hamiltonian (1), one can obtain the exact expressions of these Green’s functions using equation of motion approach. From the relations between the Green’s functions and the correlation functions [16], we obtain the thermoelectric power as

$$S_T = \frac{1}{eT} \sum_k \frac{(\Delta_{k_x} t_{k}^2)|\langle t_{k} - B \mu B \tanh(\beta B \mu B) \rangle|}{4 \cosh^2(\frac{\beta B \mu B}{2})} - \mu)$$

(11)

It should be noted that the above expression for the thermoelectric power is an exact expression for the infinite U Hubbard model. It is valid in all dimensions. Other approaches for the transport properties for the infinite U, based on usual fermions, do not give the exact expression for the thermoelectric power, except in one dimension [5]. In atomic as well as high temperature limits ($t_{k}/T \rightarrow 0$), the above expression reduces to a very simple expression

$$S_T = -\frac{k}{e} \ln\left(\frac{n}{1-n}\right) - \ln(2 \cosh(\beta B \mu B)) + \beta B \mu B \tanh(\beta B \mu B)$$

(12)

The above expression has been obtained by Mukerjee [17] for the infinite U Hubbard model in one dimension in presence of magnetic field. However, it is valid in all dimensions. First
term on the right hand side represents the Heikes formula for the spinless fermions and the second and third terms correspond to the contributions due to free spins. Thus again, we see that for the infinite U spin and charge are separated in all dimensions. Eqn. (12) can be considered as the generalized Heikes formula in presence of a magnetic field for fermions which avoid double occupancy. In low temperature limits, it is easy to show that the general expression (11) reproduces the results of Stafford [6] in one dimension. Also in one dimension, in absence of a magnetic field, it reduces to the exact expression of Kwak and Beni [5]. Recently Shastry[18] has gone beyond atomic limit and have obtained an approximate expression of thermoelectric power up to first order in the nearest neighbor transfer integral, $t_{k}$. However, from Eqn. (11), we can calculate the thermoelectric power for all values of $t_{k}$. At present this program is being carried out.

4. Conclusions
We have studied several thermodynamic and transport properties like specific heat, entropy, magnetization, magnetic susceptibility and thermoelectric power for the non-interacting orthofermions which represent the infinite U Hubbard model. It is found that in one dimension our results coincide with that of known exact results and there is a spin charge separation in all dimensions. In case of thermoelectric power, we have also obtained the generalized Heikes formula in high temperature limits and stafford results [6] at low temperatures. Since the non-interacting orthofermion model is exactly solvable in any dimension, our results can be used as a guide to ascertain the accuracy of the approximations, used to solve the finite U Hubbard model. At present, we are doing numerical calculations for all the above discussed thermodynamic and transport properties for various forms of single particle energy $t_{k}$. For parabolic type dispersion of $t_{k}$, we shall compare our results with that of free fermions in one, two and three dimensions. For lattice structures, we shall consider cubic and triangular lattices and shall compare our results with the known experimental and theoretical results in $NaCo_2O_4$ and other strongly correlated electron systems.

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