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Specific Heat of the 2D Hubbard Model: QUEST Approach.

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Abstract

The specific heat was studied as a function of temperature within the two – dimensional Hubbard model with various values of the on-site Coulombic repulsion U ranging from 2 to 16 using the Quantum Electron simulation Toolbox (QUEST) approach at half-filling. Two distinct features were identified: (1) A low temperature peak appeared when the low lying spin states are excited, and (2) a higher temperature broad peak appeared when states in the upper Hubbard band are excited. It was also observed that in the weak coupling regime the low temperature peak moves to slightly higher temperature as U increases, reaching a turning point at U≈ 11.

Keywords: strongly correlated electrons; superconductivity; specific heat; half-filling; coupling regime; on-site Coulombic repulsion.

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1.0 Introduction

The Hubbard model is among the simplest Hamiltonians that describes the behavior of correlated electrons. In spite of the considerable effort that has been devoted to the search for superconducting long-range correlations in models of strongly interacting electrons, no clear indications of their existence have been found in the realistic regime of parameter space [1- 3].

In the simplest form, the Hubbard model first introduced to describe the correlations of electrons in a narrow d-band of transition metals, contains a kinetic term which describes the motion of the electrons among the sites of the Bravais lattice and an interaction term between electrons of opposite spin on the same lattice site. By varying the model parameters, it is believed that the Hubbard Hamiltonian is applicable to describe the metal – insulator transition in a series of transition metal oxides such as $Sr_{1-x}\ La_x\ T_i\ 0_3$ [4, 5].

Specially since the discovery of high temperature superconducting materials, considerable attention has been devoted to this model and significant progress was achieved in understanding its ground state properties, particularly at half – filling, although superconductivity is still elusive. However, not much attention has been given to its thermodynamic properties despite the large amount of experimental measurements on the specific heat for the cuprates.

Even in the simplest case, definitive results have been difficult to obtain. Some exact results are available for one-dimensional systems. Lieb and Wu [6] obtained an exact expression for the ground-state energy of a one-dimensional system in the half – filled band case. The ground state is antiferromagnetic although it lacks long-range order, and insulating for any nonzero U. The excited states of this system were studied by Ovchinnikvo [7], who described spin-wave states and quasi-ionic states. The magnetic susceptibility at T = 0 was calculated by Takahashi [8]. The Hubbard model with nearest – neighbour hopping and one type of orbital applied to small clusters, with emphasis on an octahedron (six sites) was studied by Callaway et al [9]. Also in that work, the complete eigenvalue spectrum was calculated, the thermodynamic properties

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were computed with the use of a canonical ensemble and results were reported for the specific heat, spin susceptibility, and spin-spin correlation functions. The aim of this paper is to present a theoretical study of the specific heat of the two dimensional Hubbard model for different couplings u/t and temperatures using Quantum Electron Simulations Tool box (QUEST).

The two-dimensional Hubbard Hamiltonian is

$$H = -t\sum_{\langle i,j\rangle}\left(C^{+}_{i\sigma}C_{j\sigma} + C^{+}_{j\sigma}C_{i\sigma}\right) + U\sum_{i}\left(n_{i\uparrow} - \frac{1}{2}\right)\left(n_{i\downarrow} - \frac{1}{2}\right) - \mu\sum_{i}\left(n_{i\uparrow} + n_{i\downarrow}\right) \tag{1.1}$$

Here $C^{+}_{i\sigma}\left(C_{j\sigma}\right)$ are creation (destruction) operators for a Fermion of spin σ on lattice site *i* and $\langle i, j\rangle$ indicates that the sum on a two-dimensional square lattice is over pairs of nearest neighbour. U is the on-site Coulombic repulsion, t the nearest neighbour hopping amplitude, and μ the chemical potential.

2.0 General Formulas for the Electronic Specific Heat [3]:

The specific heat $C(T)$ is defined as

$$C(T) = \frac{dE}{dT} \tag{2.1}$$

where E is the internal energy density, given by the thermal average of the Hamiltonian

$$E = \frac{1}{N}\langle H\rangle \tag{2.2}$$

N being the number of sites. Calculation of internal energy by means of equation (2.2) will generally requires the calculation of two-particle Green's functions. An alternative way to calculate the internal energy is the following. By introducing the Helmholtz free energy per site

$$F = E - Ts \tag{2.3}$$

where s is the entropy per site. From the thermodynamics we have

$$S = -\left(\frac{\partial F}{\partial T}\right)_{n},\ \mu = \left(\frac{\partial F}{\partial n}\right)_{T},\ \left(\frac{\partial S}{\partial n}\right)_{T} = -\left(\frac{\partial \mu}{\partial T}\right)_{n} \tag{2.4}$$

Then, it is straight forward to obtain the following formulas

$$F(T,n) = \int_{0}^{n}\mu(T,n')\,dn' \tag{2.5}$$

$$S(T,n) = -\int_{n}^{n}\left(\frac{\partial \mu}{\partial T}\right)_{n'}dn' \tag{2.6}$$

$$E(T,n) = \int_{0}^{n}\left[\mu(T,n') - T\left(\frac{\partial \mu}{\partial T}\right)_{n'}\right]dn' \tag{2.7}$$

From which the specific heat turns out to be

$$C(T,n) = -T\int_{0}^{n}\left(\frac{\partial^{2}\mu}{\partial T^{2}}\right)n'\,dn' \quad [3] \tag{2.8}$$

In this scheme the thermodynamic quantities are all expressed through the chemical potential whose determination requires knowledge of the single – particle Green's function.

For the purpose of this work, we consider the specific heat as a function of temperature by the use of QUEST. The results obtained agreed favourably well with the works of Duffy et al [1], Mancini et al [3] and Bonca et al [10].

3.0 Results

In fig. 1a – 1g, specific heat versus temperature at half-filling for different values of U is shown. There are two important features in these curves: (1) A low temperature peak that appears when the low lying spin states are excited, and (2) a higher temperature peak which appears when states in the upper Hubbard band are excited. In the weak coupling regime the low temperature peak moves to slightly higher temperature as U increases, reaching a turning point at U ≈ 11, while in the works of Duffy and Moreo [1], the turning point is at U ≈ 7 using Quantum Monte Carlo technique.

The graphs of the specific heat versus temperature for the various values of U are presented in Figs. 1a – 1h.

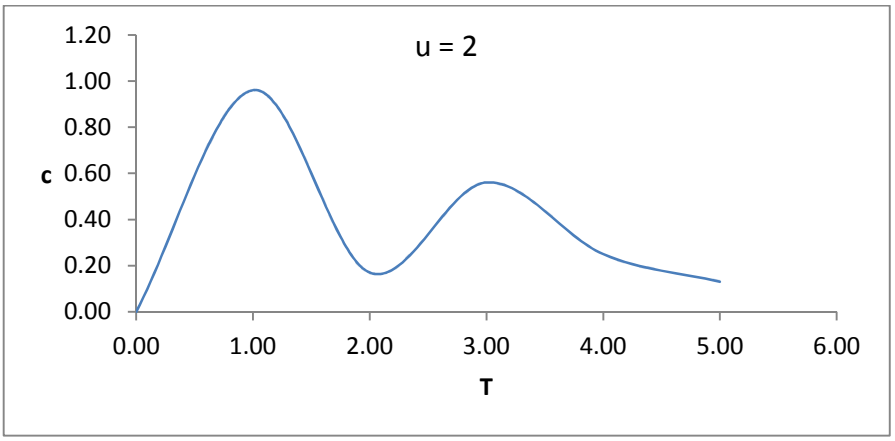

Fig.1a: Specific heat c versus temperature T on a 6x6 cluster at half-filling when $\mu = 0$, $\rho = \langle n \rangle = 1.0$ for U = 2.

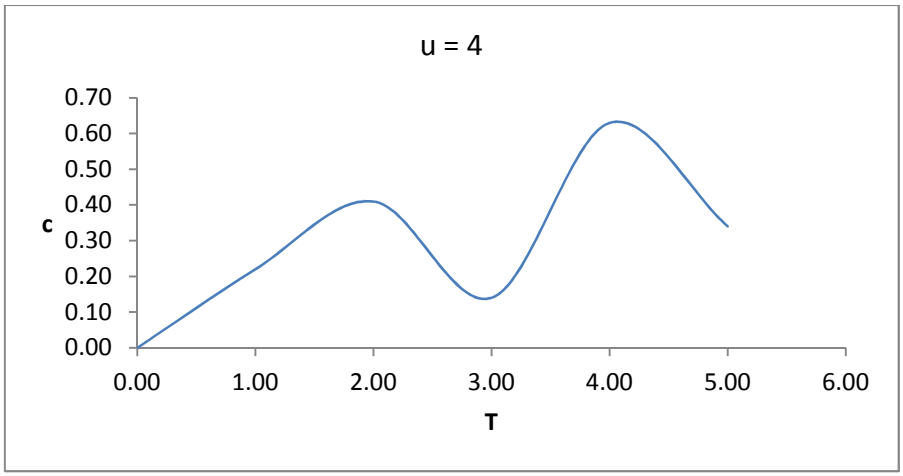

Fig.1b: Specific heat c versus temperature T on a 6x6 cluster at half-filling when $\mu = 0$, $\rho = \langle n \rangle = 1.0$ for U = 4.

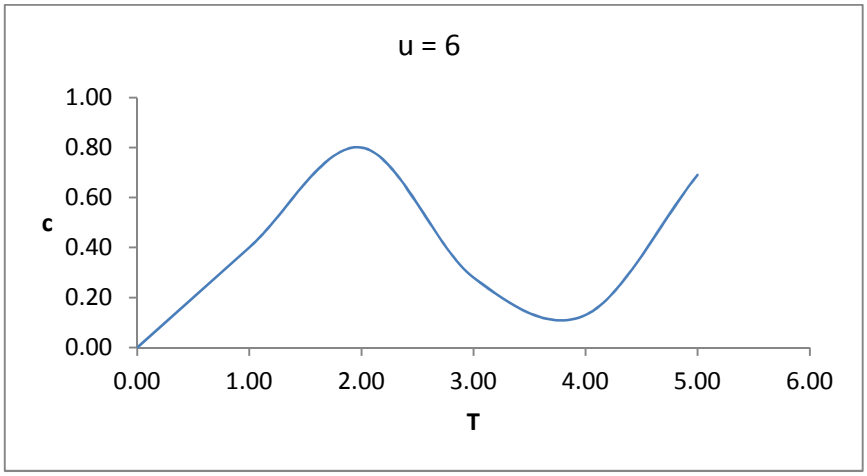

Fig.1c: Specific heat c versus temperature T on a 6x6 cluster at half-filling when $\mu = 0$, $\rho = \langle n \rangle = 1.0$ for U = 6.

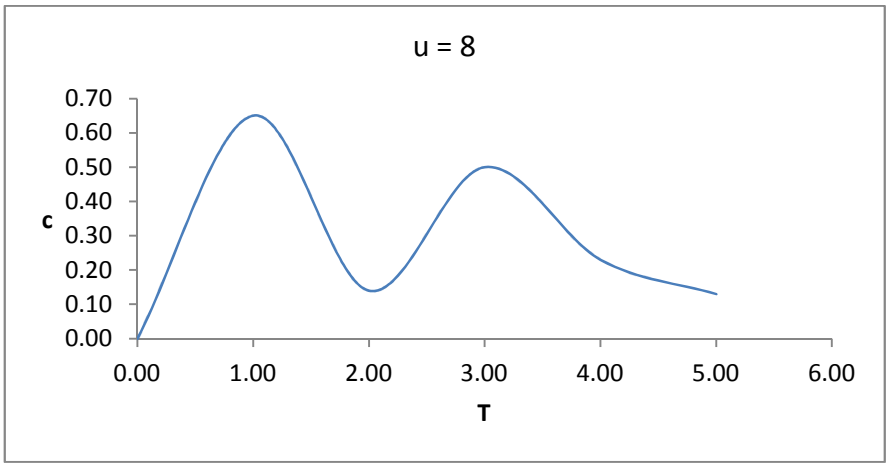

Fig.1d: Specific heat c versus temperature T on a 6x6 cluster at half-filling when $\mu = 0$, $\rho = \langle n \rangle = 1.0$ for U = 8.

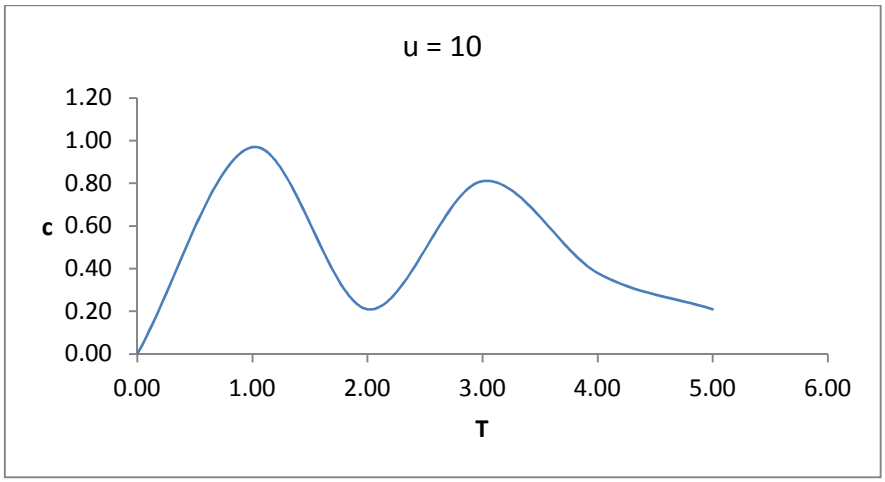

Fig.1e: Specific heat c versus temperature T on a 6x6 cluster at half-filling when $\mu = 0$, $\rho = \langle n \rangle = 1.0$ for U = 10.

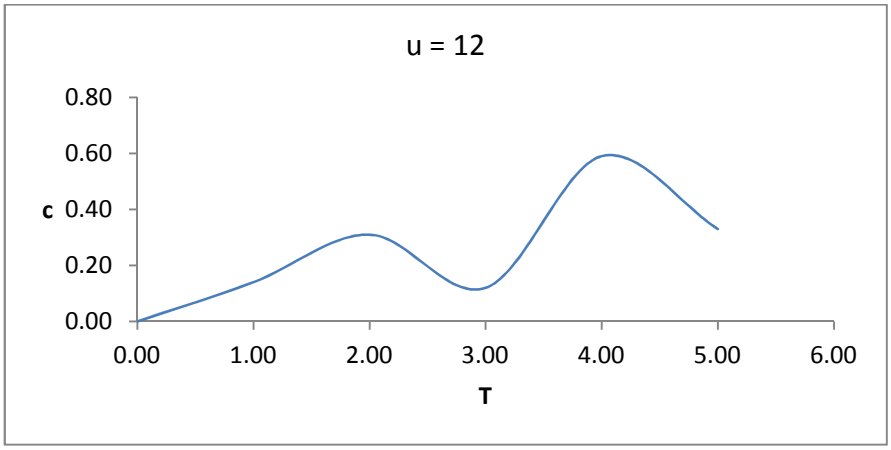

Fig.1f: Specific heat c versus temperature T on a 6x6 cluster at half-filling when $\mu = 0$, $\rho = \langle n \rangle = 1.0$ for U = 12.

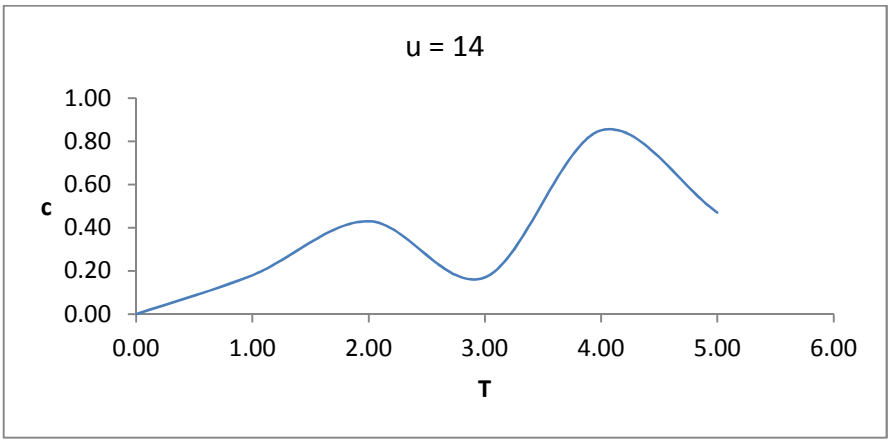

Fig.1g: Specific heat c versus temperature T on a 6x6 cluster at half-filling when $\mu = 0$, $\rho = \langle n \rangle = 1.0$ for U = 14.

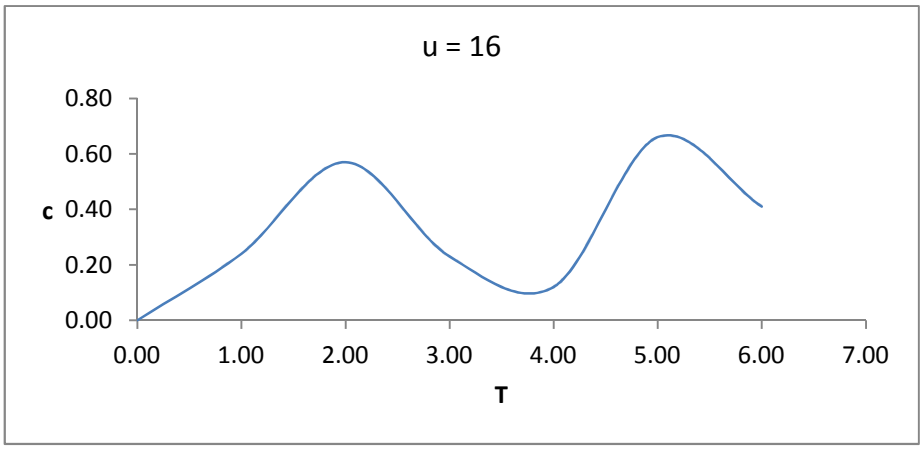

Fig.1h: Specific heat c versus temperature T on a 6x6 cluster at half-filling when $\mu = 0$, $\rho = \langle n \rangle = 1.0$ for U = 16.

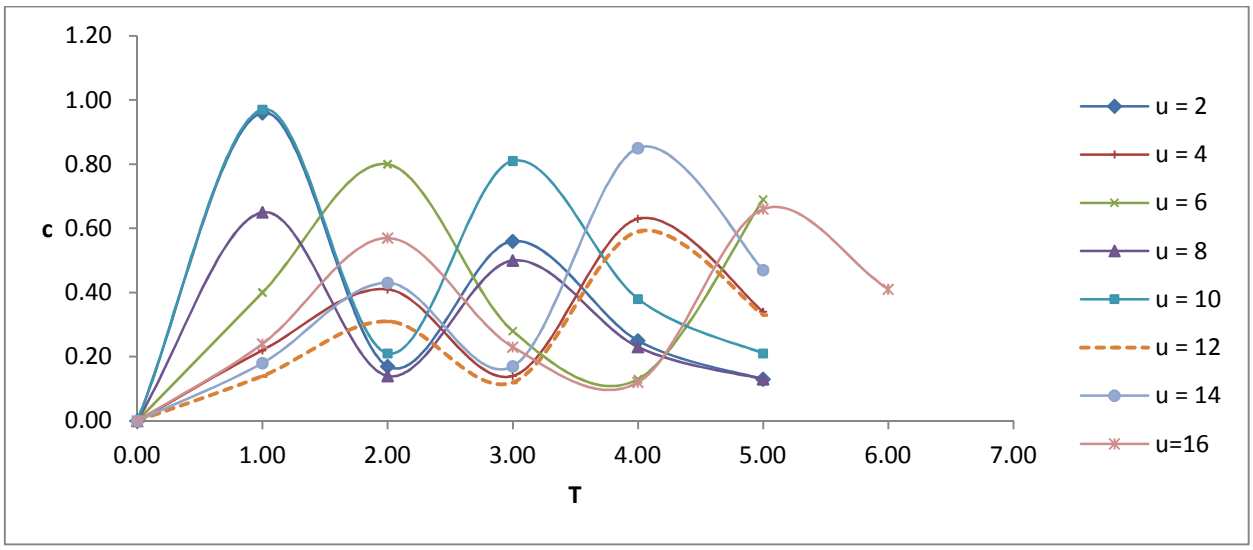

Fig.2: Combination of all the couplings of Specific heat c versus temperature T on a 6x6 cluster at half-filling when $\mu = 0$, $\rho = \langle n \rangle = 1.0$ for the different values of U ranging from 2 to 16.

4.0 Conclusion

The specific heat of the two – dimensional Hubbard model has been calculated using QUEST approach for different couplings as a function of temperature at half – filling. As the coupling U increases a low temperature peak associated with spin degrees of freedom moves to lower temperatures, while a high temperature peak associated with the charge degrees of freedom moves to higher temperatures. These features are in agreement with [1, 3, 10].

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