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A Study Of The Internal Energy And Magnetic Spin Susceptibility Of The 2-D Hubbard Model Representation Of High Temperature Superconductors Via An Exact-Approach

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Abstract

An exact approach is re-visited in performing a comparative analysis of the attractive and repulsive 2-D Hubbard model (AHM and RHM respectively) which is used in describing a simplified 2x1 (Cu-O-Cu) lattice (known to play significant role in HT_c-superconductivity in cuprates) with the use of the MATLAB. The response of the temperature-dependent internal energy, E(kT), to the simultaneous variation of both the on-site interaction and the nearest-neighbour hopping integral (U,t) shows that HT_c-superconducting materials described by the AHM are not only more stable but sustain their stable state over a relatively wider temperature range. The spectrum of the magnetic spin susceptibility, $\chi(T)$, reveal certain interesting character which are used to account for various observed phenomena in HT_c-superconducting materials (like the coexistence of charge density wave (CDW) and spin density wave (SDW) in the semiconducting phase of $Ba_{1-x}K_xBiO_3$ and $BaPb_xBi_{1-x}O_3$. Furthermore, various correlations are suggested while the outer limits of the critical values of U for pair formation and associated spin gap, U_p=-2eV for AHM and 3eV for RHM. Results obtained are also in strong agreement with results of QMC simulations for more realistic 3-band Hubbard model among others.

1.0 Introduction

One of the salient hindrances in the search for an appropriate Hamiltonian that may adequately represent a generally acceptable theory of high-temperature (HT_c)-superconductivity lies with the mathematical/analytical tool(s) applied in the evaluation of these theoretical proposals (which in general, determines the potency of any proposed Hamiltonian). A major problem in the numerical simulation of many-electron systems is the inability to carry out calculations at sufficiently low temperatures [23]. This is attributed to the wide range of fermion matrix eigenvalues which create considerable difficulty in the numerical evaluation of the determinant or inverse of the fermion matrix. Moreover, some algorithms earlier developed which allow simulation to be carried out within the grand canonical ensemble at low temperature tend to be slow at low temperature due to a resulting rapid growth of the computer time needed.

It is instructive [8] to study simplified models that display the essential features of High-Temperature Superconductors (HTS) in the search for the mechanism responsible for HT_c-superconductivity. A model that had been used most frequently to discuss the possibility for superconductivity in strongly correlated systems is the Hubbard model (HM) [11, 16]. As a matter of fact, it is seen as a good starting point for the

theoretical understanding of HT_c-superconductivity [13]. However, numerous methods that had been applied for the numerical analysis of the HM are generally very complex and many-a-time require some degree of approximation/assumptions; some of which are faulty, making difficult the clear understanding of the physical consequences.

It has been demonstrated [3] that an exact solution is an effective prescription for solving model Hamiltonian like the Hubbard, t- J and pseudo-Hubbard models, in comparison to perturbation or approximate methods like the mean-field (finite-temperature) Gutzwiller variational scheme and the Quantum Monte Carlo simulations for strongly correlated electron gas; where there are indications that the exact solution has the essential physical aspect of the problem. However, the degree of success of earlier attempts at the exact approach was hampered by the tools employed for analysis (like the FORTRAN), which apart from an initial mathematical manipulation that had to be done rigorously, also involved very complex programming. These were compounded by the difficulty in handling equations involving exponential matrix functions, whose computational complexity grows with the increase in the matrix dimension, and a further difficulty in its application at very low temperatures.

In this paper, the MATLAB is applied in a study of the temperature-dependent internal energy, *E(kT)* and the magnetic spin susceptibility $\chi(T)$ of HTS using an exact method and fundamental principles/basic formulae, thereby eliminating errors that otherwise may be introduced by any form of approximation or mathematical/computational manipulation. The system of interest here is the simplified superconducting CuO_2 plane of two sites, a 2x1 (Cu-O-Cu) lattice that play very important role in HT_c-superconductivity in cuprates. Actually, it is generally believed that the mechanism for HT_c-superconductivity in cuprates lie within the CuO_2 planes [6, 21] where a Cu-O-Cu angle of 180^o is favourable for HT_c superconductivity.

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2.0 THE EXACT METHOD

The 2-D Hubbard Hamiltonian at ½-filling (μ=0), H_H, which has been shown "Enugu group", [1, 4] to be equivalent to a transformed BCS Hamiltonian in Wannier representation, H_{BCS}^T, is given by:

$$H_H \equiv H_{BCS}^T = -t \sum_{<i,j>\sigma} \left(c_{i\sigma}^+ c_{j\sigma} + c_{j\sigma}^+ c_{i\sigma} \right) + U \sum_{i(j)} n_{i\uparrow} n_{i\downarrow} \qquad (2.1)$$

where t is the strength of the nearest-neighbor (nn) hopping which is determined by the overlapping integral between the two sites; U is the intra-atomic Coulomb interaction; n_i, the number operator; $c_{i(j),\sigma}^+$ and $c_{i(j),\sigma}$ are the creation and annihilation operators respectively.

This equivalence promises the use of modified versions of the standard BCS model [5] for the study of high-temperature superconductors (HTS) in order to explain not only the coexistence of superconductivity and antiferromagnetism, but the rich variety of the properties of the HT_c-materials [4]. The interest in the 2-D Hubbard model is based on the possibility that the competition between the kinetic energy and the Coulomb energy gives rise to strong electron correlation which may be relevant to HT_c-superconductivity. Due to the proximity of antiferromagnetic and superconducting phases, Coulomb correlations can be considered as a possible non-phononic mechanism of HT_c-superconductivity [22].

Following the lead introduced originally by [22], which was later adapted by [1] and [3], the creation and annihilation operators in a 4-fermion system are represented by 2^4x2^4 (i.e. 16x16) matrices extracted from the 16 many-electron states that form the basis for the representation of the system (Table 1; after [3]):

Table 2.1: The 16 basis many-electron states of a 4-fermion system

INDEX	STATE	REMARK
0	Vacuum	0-particle state
1	$\left\|i=1,\uparrow\right\rangle$	1-particle state
2	$\left\|i=1,\downarrow\right\rangle$	”
3	$\left\|i=2,\uparrow\right\rangle$	”
4	$\left\|i=2,\downarrow\right\rangle$	”
5	$\left(\left\|i=1,\uparrow\right\rangle,\left\|i=1,\downarrow\right\rangle\right)$	2-particle state
6	$\left(\left\|i=1,\uparrow\right\rangle,\left\|i=2,\uparrow\right\rangle\right)$	”
7	$\left(\left\|i=1,\uparrow\right\rangle,\left\|i=2,\downarrow\right\rangle\right)$	”
8	$\left(\left\|i=1,\downarrow\right\rangle,\left\|i=2,\uparrow\right\rangle\right)$	”
9	$\left(\left\|i=1,\downarrow\right\rangle,\left\|i=2,\downarrow\right\rangle\right)$	”
10	$\left(\left\|i=2,\uparrow\right\rangle,\left\|i=2,\downarrow\right\rangle\right)$	”
11	$\left(\left\|i=1,\uparrow\right\rangle,\left\|i=1,\downarrow\right\rangle,\left\|i=2,\uparrow\right\rangle\right)$	3-particle state
12	$\left(\left\|i=1,\uparrow\right\rangle,\left\|i=1,\downarrow\right\rangle,\left\|i=2,\downarrow\right\rangle\right)$	”
13	$\left(\left\|i=1,\uparrow\right\rangle,\left\|i=2,\downarrow\right\rangle,\left\|i=2,\downarrow\right\rangle\right)$	”
14	$\left(\left\|i=1,\downarrow\right\rangle,\left\|i=2,\uparrow\right\rangle,\left\|i=2,\downarrow\right\rangle\right)$	”
15	$\left(\left\|i=1,\uparrow\right\rangle,\left\|i=1,\downarrow\right\rangle,\left\|i=2,\uparrow\right\rangle,\left\|i=2,\downarrow\right\rangle\right)$	4-particle state

Shown below are 4 explicit 16x16 matrix representations of the annihilation operators, $c_{1\uparrow}, c_{1\downarrow}, c_{2\uparrow}$ *and* $c_{2\downarrow}$, from which the corresponding creation operators $c_{1\uparrow}^{+}, c_{1\downarrow}^{+}, c_{2\uparrow}^{+}$ *and* $c_{2\downarrow}^{+}$ can be deduced. Off-course, these operators satisfy the usual anticommutation relations:

$$\left.\begin{aligned} \left\{c_{i\sigma}^{+}, c_{j\sigma'}\right\} &= \delta_{ij}\delta_{\sigma\sigma'} \\ \left\{c_{i\sigma}^{+}, c_{j\sigma}^{+}\right\} &= \left\{c_{i\sigma}, c_{j\sigma}\right\} = 0 \end{aligned}\right\} \tag{2.2}$$

$$c_{1\uparrow} = \begin{vmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{vmatrix} \tag{2.3}$$

$$c_{1\downarrow} = \begin{vmatrix} 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{vmatrix} \tag{2.4}$$

$$c_{2\uparrow} = \begin{vmatrix} 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{vmatrix} \tag{2.5}$$

$$c_{2\downarrow} = \begin{vmatrix} 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{vmatrix} \tag{2.6}$$

The MATLAB is now programmed to obtain the matrix representation of $H_{BCS}^{T} \equiv H_{H}$ in equation (2.1) by the substitution of expressions (2.3) to (2.6):

$$H_{BCS}^{T} = \begin{pmatrix}
0 & & & & & & & & & & & & & & & \\
 & 0 & 0 & -t & 0 & & & & & & & & & & & \\
 & 0 & 0 & 0 & -t & & & & & & & & & & & \\
 & -t & 0 & 0 & 0 & & & & & & & & & & & \\
 & 0 & -t & 0 & 0 & & & & & & & & & & & \\
 & & & & & U & 0 & -t & t & 0 & 0 & & & & & \\
 & & & & & 0 & 0 & 0 & 0 & 0 & 0 & & & & & \\
 & & & & & -t & 0 & 0 & 0 & 0 & -t & & & & & \\
 & & & & & t & 0 & 0 & 0 & 0 & t & & & & & \\
 & & & & & 0 & 0 & 0 & 0 & 0 & 0 & & & & & \\
 & & & & & 0 & 0 & -t & t & 0 & U & & & & & \\
 & & & & & & & & & & & U & 0 & t & 0 & \\
 & & & & & & & & & & & 0 & U & 0 & t & \\
 & & & & & & & & & & & t & 0 & U & 0 & \\
 & & & & & & & & & & & 0 & t & 0 & U & \\
 & & & & & & & & & & & & & & & 2U
\end{pmatrix} \tag{2.7}$$

This is a symmetric diagonal matrix in "Jordan's Canonical form" [9] with three identifiable "Blocks". All off-Block entries are zeros. The matrix diagonalization is automatically done by MATLAB.

3.0 Internal Energy And Magnetic Spin Susceptibility

The Hamiltonian

$H_{BCS}^{T} \equiv H_H = H$

obtained in equation (2.7) as a symmetric diagonal 16x16 matrix in "Jordan's Canonical form" represents an excellent testing ground for the exact method with the use MATLAB. Not only are the physical properties of this model of great interest [23], there are also a variety of results available for comparison.

The grand quantum partition function, z, is given by [25]

$$z = Tr\left(e^{-\beta H}\right) \tag{3.1}$$

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

The temperature-dependent internal energy, *E(kT)* is derived from *z*:

$$E(kT) = -\tau^2 \frac{\partial\left(F/\tau\right)}{\partial\tau} \tag{3.2}$$

where

$$F(T) = -\tau \log(z) \tag{3.3}$$

is the temperature-dependent Helmholtz free energy,

and

$$\tau = 1/\beta; \tag{3.4}$$

while the temperature-dependent magnetic spin susceptibility, $\chi(T)$ is calculated from

$$\chi(T) = \left\langle \frac{\left[N^{-1}\sum_i \left(n_{i\uparrow} - n_{i\downarrow}\right)\right]^2}{T} \right\rangle \tag{3.5}$$

with *N* being the number of fermions.

The thermal average of an operator $\hat{O}$ is defined if $\hat{O}$ is expressed in terms of fermion creation and annihilation operators, and can be calculated from $\left\langle \hat{O} \right\rangle = Tr\left(\frac{\hat{O}e^{-\beta H}}{z}\right)$

(3.6)

4.0 Comparative Analysis

The MATLAB is applied in numerically studying the responses of the above defined temperature-dependent internal energy, *E(kT)*, and the magnetic spin susceptibility, $\chi(T)$, to various values of (*U,t*) involving exponential functions of the 16x16 matrix representations of the creation/annihilation operators and the Hubbard Hamiltonian for both the Attractive 2-D Hubbard model (AHM) i.e with U<0, and the Repulsive 2-D Hubbard model (RHM) with *U*>0 (for μ=0), over the range 0.1eV≤ *kT* ≤5.0eV at intervals of 0.02eV (which ensures high resolution of the results even at low temperatures). In this work we take *k*=1 where *F(T)* had earlier been evaluated [1, 2]. The range –10eV≤*U*≤10eV is chosen while the corresponding *t* is either 1eV or 0.43eV so as to be within the order of known experimental values at half-filling [12], Table 4.1:

Table 4.1 : Pair-values of (*U,t*):

***U*/eV**	-10.0	-5.0	-4.0	-0.137	0.0	0.137	4.0	5.0	10.0

***t*/eV**	1.0	0.43	1.0	0.43	1.0	0.43	1.0	0.43	1.0

Internal Energy, *E(kT)*

Two distinct sets of curves distinguishing those for AHM from those belonging to RHM, for the internal energy, *E(kT)*, as a function of temperature and in response to various values of (*U*,t) are displayed in Figure (1).

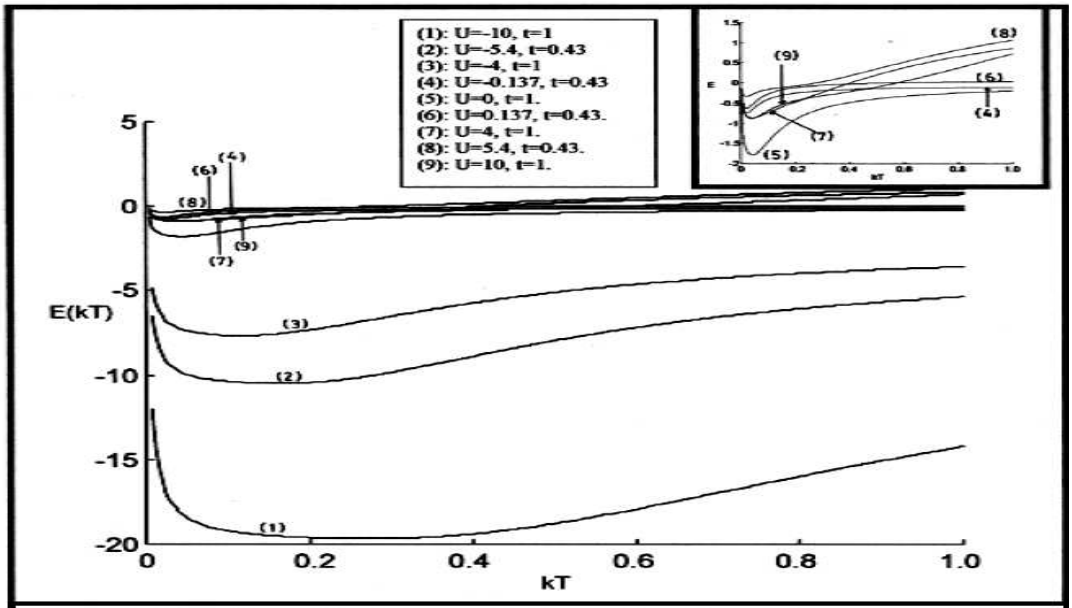

Figure 1: The effect of both the on-site interaction, *U*, and the nearest-neighbour hopping integral, *t*, on the internal energy, *E(kT)*. Insert shows the relatively fast drop in *E(kT)* at very low temperature in the repulsive Hubbard model

The curves for AHM curves show marked variation of *E(kT)* with (*U*,*t*);while those for the RHM form a much more closely packed set of curves which cross each other. Generally, the AHM curves have lower internal energy; suggesting a higher stable state. However, *E(kT)* has negative values for both aspects of the model.

Furthermore, for all (*U*,*t*), as *T* increases from 0^{o}K, *E(kT)* decreases to a minimum, E_{min}, then rises smoothly to approximately its initial value at higher temperatures. The E_{min}, for the RHM, has a smaller half-width (see insert of

Figure (1)) than those of the AHM whose E_{min} are spread over a wider temperature range. This suggests that HT_c-

superconducting materials described by the AHM may not only be more stable but may sustain their stable state over a wider temperature range.

Magnetic Spin Susceptibility, $\chi(T)$

The curves (see figure 2) for the RHM has excellent agreement with those of undoped $La_{1.85}Sr_{0.15}Cu_{1-x}M_xO_{4-y}$, which exhibits Pauli as well as Van Vleck paramagnetic contribution; and at higher temperatures, a Curie-Weiss type of behavior is noticed, which is similar to the behavior induced,

with both Ni and Zn doping of $La_{1.85}Sr_{0.15}Cu_{1-x}M_xO_{4-y}$, where the effective moments may be determined to fit

$$\chi(T) = \frac{C}{(T+\theta)} + \chi_o \tag{4.1}$$

where C and θ are the Curie constant and Curie temperature respectively [14].
This may show a slight positive temperature coefficient of χ which may be interpreted as a tail of a broad maximum at a higher temperature resulting from a short-ranged antiferromagnetic correlation in the 2-dimensional sheets of CuO_2 [8, 10, 14, 18, 19, 20].

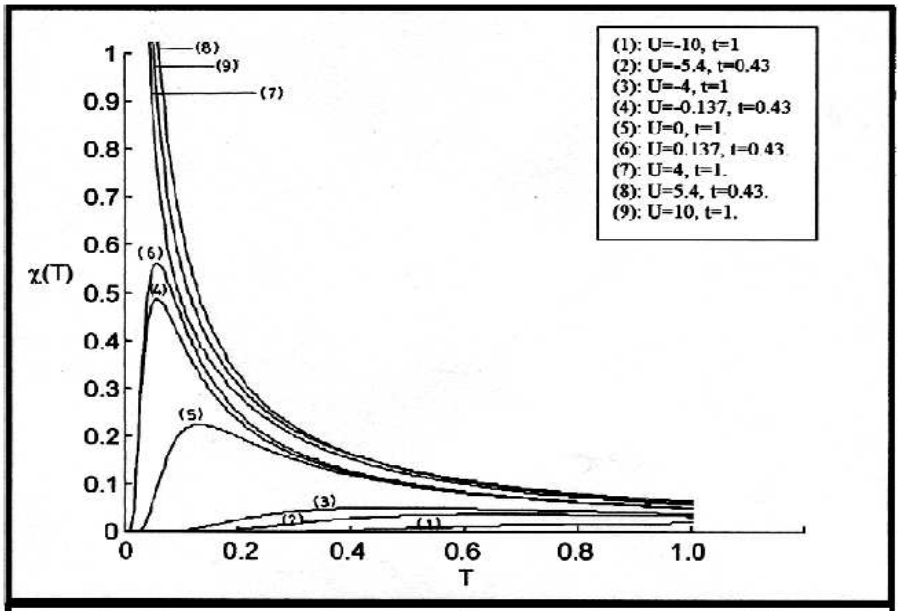

Figure 2: The temperature-dependent uniform magnetic spin susceptibility, $\chi(T)$ for different values of the on-site interaction, U, and the nearest-neighbor hopping integral, t.

Another inference [19] of the Curie-like paramagnetic contribution is that, in $Ba_{1-x}K_xBiO_3$ and $BaPb_xBi_{1-x}O_3$, this could be a spin density wave (SDW) domain wall between the charge density wave (CDW) domain with discontinuing phases by considering 1- or 2-dimensional models i.e. the coexistence of the CDW and SDW is suggested in their semiconducting phase.
The trend of χ(T) for RHM is also similar to that which demonstrates the temperature-dependence of the higher critical field, H_{c2} [14, 15], pointing to a possible correlation of U and H_{c2}. On the other hand, there seem to be a correlation between doping, δ, and U for $U \leq 0$ (i.e AHM) when χ(T) in Figure (2) is compared with the temperature-dependence of χ in a constant field of 1T of $Pb_2Sr_2Y_{1-x}Ca_xCu_3O_{8+\delta}$ (which is very similar to those of other HT_c-superconductors (HTS) with pyramidal CuO_2 layers such as $Bi_2Sr_2Ca_{1-x}Y_xCu_2O_{8+\delta}$ (where these pyramidal CuO_2

layers may control almost all the properties of these HT_c-materials including their transition temperature, T_c). This correlation between doping, δ, and U, and the general trends of our results, are in strong agreement with results of QMC simulations for the more realistic 3-band Hubbard model [7, 8].

While the peaks in Figure (2) are a clear signature of the antiferromagnetic ordering of Cu^{2+} spins in HTS as is clearly detected in $La_{2-x}Ba_xCuO_4$ [14, 18, 24], the suppression in χ

for the AHM is generally below some temperature, $T^x(U)$. This suppression can be understood in the strong-coupling regime by noticing that local pairs are being formed, and that spin excitations necessarily imply pair breaking with an energy cost (gap) of the order $|U|$. The formation of local pairs and the associated spin gap should be reflected in the magnetic properties (this line of reasoning could be applied for intermediate coupling). $T^x(U)$ may thus represent a crossover temperature separating two normal-state regions: metallic and spin gap. It could be inferred, therefore, that pair formation can only occur below a critical value of $U=U_p$. For AHM, $U_p \in$ (-2eV, -1eV] which begins at the temperature where $\chi(U=0) = \chi(U=-1)$; while for RHM, $U_p \in$ [2eV, 3eV) beginning at the temperature where $\chi(U=0.137) = \chi(U=2)$. Our range of U_p for RHM is smaller than the value predicted by [17] i.e. $U_p \sim 7.8$eV, within a low-density approximation; while our result for AHM agrees with that obtained by [8], $U_p \in$ [-2, -1] through Quantum Monte Carlo (QMC) simulation in his work on 3-dimensional attractive Hubbard model. Our results may be taken as the outer limits for all HTS.

SUMMARY AND CONCLUSION

The 2-D Hubbard model is used to represent the Cu-O-Cu lattice which is known to play important role in HT_c-superconductivity in cuprates where a Cu-O-Cu angle of 180^o had been established as being favourable for HT_c-superconductivity. An exact approach which led to a 16x16 matrix representation of the 2-D Hubbard Hamiltonian in Jordan's canonical form is used (with the application of MATLAB) to study the effects of simultaneously varying (U,t) on the temperature dependent $E(kT)$ and χ(T). This comparative study is done for both the AHM and RHM which included their respective intermediate and strong coupling limits.

The response of $E(kT)$ with changes in (U,t) suggests that HT_c-superconducting materials described by the AHM may not only be more stable but may sustain their stable state over a wider temperature range.

The analysis of χ(T) further confirms earlier reports of paramagnetic and antiferomagnetic signatures obtained in an exact broad-spectrum analysis of the Helmholzt free energy, $F(T)$, and the entropy of 2-D Hubbard Hamiltonian representation of HTS [2]. The results obtained are used in accounting for various separately observed properties/phenomena of HT_c-superconducting materials. Furthermore, a correlation between U and Hc_2 in RHM and between δ and U in AHM are suggested. Finally, outer limits for the critical values of U below which the formation of local pairs and the associated spin gap occur, U_p, are deduced as -2eV for AHM and 3eV for RHM.

The results obtained well account for various experimental observations and compare favorably with more sophisticated and realistic models and known analytical methods. This work, as in an earlier analysis, further suggests that the inadequacies of known numerical methods/tools might have greatly inhibited the inability to achieve a desired model that would adequately account for HTS. The success of this exact method, with the use of MATLAB, encourages the re-evaluation of some theories that were hitherto supported by approximate analysis.

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