J. Nig. Ass. Math. Phys.
Vol. 1 (1992) 23 - 28

AN EXACT SOLUTION OF THE HUBBARD HAMILTONIAN MODEL FOR HIGH TEMPERATURE SUPERCONDUCTORS

by

C. N. Animalu
Department of Physics and Astronomy
University of Nigeria
Nsukka, Nigeria.

ABSTRACT

Using a $2^N \times 2^N$ matrix representation of the creation and annihilation operators for an N-fermion system, we present an exact diagonalization of the Hubbard Hamiltonian for a strongly correlated many-electron system. The result is applied to the thermodynamic properties and spin susceptibility of high-temperature superconductors, such as $YBa_2Cu_3O_{7-x}$ (with T_c = 90K) in which superconductivity is believed to occur in CuO_2 planes, and whose electronic structure is described by the Hubbard Hamiltonian. Effects of correlation are observed in the electronic specific heat, which are not seen in results obtained by the standard mean-field approximation method, such as the Gutzwiller variational method. The magnetic spin susceptibility compares favourably with the quantum Monte Carlo simulations of White et al. Other applications of the method to the many-body problem are discussed.

1. INTRODUCTION

Ceramic oxides have recently been synthesized, which have superconducting transition temperatures (T_c) well above 30K. Examples are $(La_{1-x}Ba_x)_2CuO_4$ with T_c = 35K, $YBa_2Cu_3O_{7-x}$ with T_c = 90K, and $Bi_2Ca_{n-1}Sr_2Cu_nO_{2n+4+x}$, n = 1, 2, or 3, with T_c = 125K, which were synthesized after 1986. $YBa_2Cu_3O_{7-x}$, where x is the oxygen concentration, has a triple perovskite crystal structure and exists in two phases: a nonsuperconducting antiferromagnetic phase $YBa_2Cu_3O_6$ and a superconducting phase $YBa_2Cu_3O_7$ (see Goodenough & Manthiram, 1988). A common feature of almost all high-temperature superconductors is the presence of CuO_2 planes in which superconductivity is believed to take place. Each copper atom is four-fold coordinated to four oxygen atoms, while each oxygen atom has two-fold coordination to two copper atoms (see figure 1a). In this arrangement, the formal valence is 2+ for copper and 2- for oxygen. Superconductivity is believed to take place when the formal valence of copper in these planes is increased slightly by doping (see figure 1b, after Zhang & Rice, 1988). In addition to high T_c's, these ceramic oxides exhibit other unusual properties, such as: (a) Negligible isotopic effect. For example, $YBa_2Cu_3O_{7-x}$ has $\beta_{Cu} = 0.0 \pm 0.07$, $\beta_{Ba} = 0.0 \pm 0.1$, and $\beta_O = 0.43$, in contrast to $\beta = 0.5$ in conv-

entional superconductors; (b) very short coherence lengths, $\xi(0) \sim 15\text{Å}$ at zero temperature (Bulaevskii et al, 1988), in contrast to $\xi(0) \sim 10^2$ to 10^4Å in conventional superconductors; (c) extremely high value of the upper critical field $\gtrsim$ 100T (Muo et al, 1988), a consequence of short coherence lengths; (d) the presence of a linear term in low-temperature specific heat (Ginsberg, 1989); and (e) the coexistence of antiferromagnetism and superconductivity (Rossat et al, 1991). Various models have been proposed, which attempt to account for these properties of high-temperature superconductors, and to determine the mechanism responsible for high-temperature superconductivity. Among these are the conventional Bardeen-Cooper-Schrieffer (BCS) theory, proposed in 1957; the Fermi liquid theory; and a theory of strong electron correlations.

In this paper, the Hubbard model of strongly correlated metals (Hubbard, 1963) for high-temperature superconductivity is solved exactly, and thermodynamic properties and magnetic spin susceptibility calculated at half-filling in a 2 x 1 lattice consisting of one copper and one oxygen site.

2. EXACT SOLUTION METHOD AND THE HUBBARD MODEL

The Hubbard Hamiltonian, in Wannier representation, is

$$H_o = -t \sum_{\langle i,j \rangle, \sigma} (c^+_{i\sigma} c_{j\sigma} + h.c) + U \sum_i n_{i\uparrow} n_{i\downarrow} - \mu \sum_i (n_{i\uparrow} + n_{i\downarrow}) \qquad (1)$$

where t is the amplitude for hopping between nearest-neighbour sites, U is the direct Coulomb interaction, μ is the chemical potential, and $c^+_{i\sigma}$ is the creation operator for an electron of spin σ at site i. This Hamiltonian, first proposed by Hubbard (1963) to explain correlation effects in transition metals, is also used to explain high-temperature superconductivity. Using a 16 x 16 matrix representation of the fermion creation and annihilation operators suggested by Thouless (1961), we obtain the following matrix H_o which corresponds to eq (1):

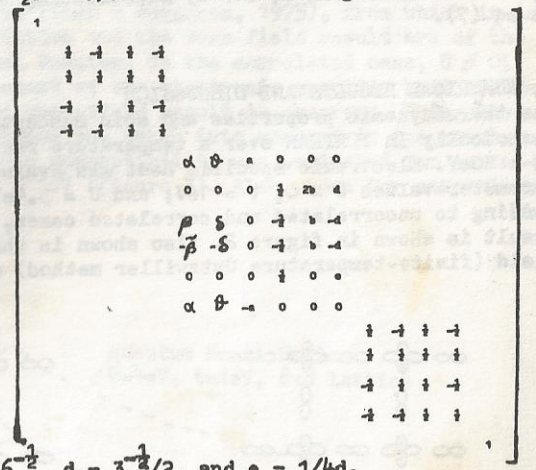
$$\begin{bmatrix}
0 & & & & & & & & & & & & & & & \\
 & A & 0 & -t & 0 & & & & & & & & & & & \\
 & 0 & A & 0 & -t & & & & & & & & & & & \\
 & -t & 0 & A & 0 & & & & & & & & & & & \\
 & 0 & -t & 0 & A & & & & & & & & & & & \\
 & & & & & -2\mu & 0 & -t & -t & 0 & 0 & & & & & \\
 & & & & & 0 & B & 0 & 0 & 0 & 0 & & & & & \\
 & & & & & -t & 0 & B & 0 & 0 & -t & & & & & \\
 & & & & & t & 0 & 0 & B & 0 & t & & & & & \\
 & & & & & 0 & 0 & 0 & 0 & B & 0 & & & & & \\
 & & & & & 0 & 0 & -t & t & 0 & -\mu & & & & & \\
 & & & & & & & & & & & 0 & 0 & t & 0 & \\
 & & & & & & & & & & & 0 & 0 & 0 & t & \\
 & & & & & & & & & & & t & 0 & 0 & 0 & \\
 & & & & & & & & & & & 0 & t & 0 & 0 & \\
 & & & & & & & & & & & & & & & -\mu
\end{bmatrix}$$

where $A = -(\mu + \frac{1}{2}U)$, $B = -(2\mu + U)$, and $C = -(3\mu + \frac{1}{2}U)$. H_o is diagonalized to give

$$H_o = \tilde{U} \Lambda_o \tilde{U}^+ \qquad (2)$$

Λ_o is the following matrix:

where $D = -(\mu + \frac{1}{2}U - t)$, $E^{\pm} = -2\mu - \frac{1}{2}U \pm \frac{1}{2}(U^2 + 16t^2)^{\frac{1}{2}}$, $F = -(2\mu + U)$, and $G = -(3\mu + \frac{1}{2}U + t)$. $\tilde{U}$ is the following matrix:



where $a = 2^{-\frac{1}{2}}$, $b = -6^{-\frac{1}{2}}$, $d = 3^{-\frac{1}{2}}/2$, and $e = 1/4d$.

3. THERMODYNAMIC PROPERTIES AND SPIN SUSCEPTIBILITY

The grand quantum partition function Z can be calculated from the diagonalization of H, and the thermodynamic properties of the Hubbard model derived from it, using

$$Z = \mathrm{Tr}(\exp(-\beta H)) = \mathrm{Tr}(\exp(-\beta \tilde{U} \Lambda_o \tilde{U}^+)) = \mathrm{Tr}(\exp(-\beta \Lambda_o)) \qquad (3)$$

where $\beta = 1/kT$ is inverse temperature. The Helmholtz free energy F, entropy S, internal energy E, and electronic specific heat C_V are derived from Z using the formulae:

$$F = -\tau \log(Z) \tag{4a}$$

$$S = -\partial F/\partial \tau \tag{4b}$$

$$E = -\tau^2 \partial (F/\tau)/\partial \tau \tag{4c}$$

$$C_V = \partial E/\partial T \tag{4d}$$

where $\tau = 1/\beta$. The thermal average of an operator R is defined if R is expressed in terms of fermion creation and annihilation operators:

$$R = \mathrm{Tr}(R\exp(-\beta H)/Z \tag{5}$$

To calculate spin susceptibility, we substitute

$$\chi(T) = \left\langle \left[N^{-1} \sum_i (n_{i\uparrow} - n_{i\downarrow})\right]^2 / T \right\rangle \tag{6}$$

for R in eq (5). Expressions for the thermodynamic properties and spin suceptibility are then:

$$Z = 1 + a + b + c + d + \exp(\beta(2\mu)) + 3e + f + g \tag{7}$$

$$\chi(T) = (\beta/4Z)\, a + b + f + g + 4e \tag{8}$$

In equations (7) and (8), $a = 2\exp(\beta(\mu + \frac{1}{2}U - t))$, $b = 2\exp(\beta(\mu + \frac{1}{2}U + t))$, $c = \exp(\beta(2\mu + \frac{1}{2}U - \frac{1}{2}(U^2 + 16t^2)^{\frac{1}{2}}))$, $d = \exp(\beta(2\mu + \frac{1}{2}U + \frac{1}{2}(U^2 + 16t^2)^{\frac{1}{2}}))$, $e = \exp(\beta(2\mu + U))$, $f = 2\exp(\beta(3\mu + \frac{1}{2}U + t))$, and $g = 2\exp(\beta(3\mu + \frac{1}{2}U - t))$. Expressions for F, S, E, and C_V are obtained from eq (4) by substituting the result for Z given in eq (7).

4. NUMERICAL RESULTS AND DISCUSSION

The thermodynamic properties and spin susceptibility were evaluated numerically in FORTRAN over a temperature range from kT = 0.1eV to kT = 10eV. Electronic specific heat was evaluated for two sets of parameter values U = 0, t = 1eV; and U = 5.4eV, t = 0.43eV, corresponding to uncorrelated and correlated cases, respectively. This result is shown in figure 2. Also shown is the result of the mean-field (finite-temperature Gutzwiller method) calculation of the

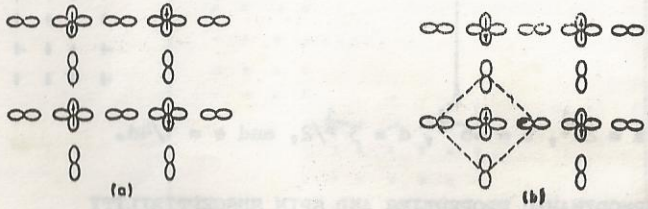


Figure 1

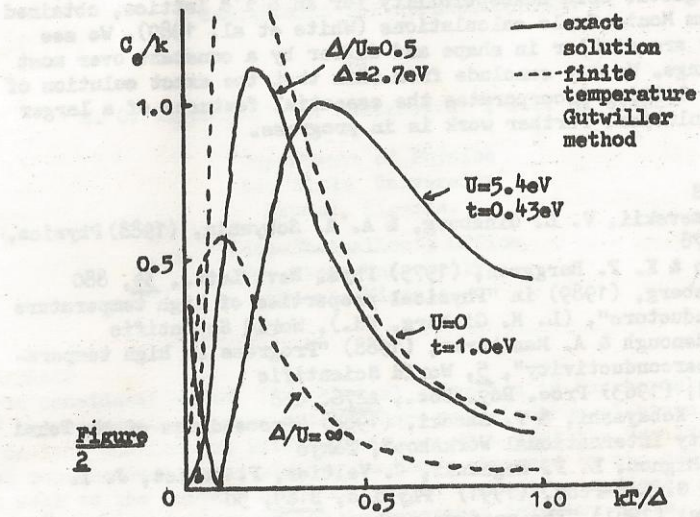


Figure 2

electronic specific heat (Chao & Berggren, 1975), from which it is seen that the exact solution and the mean-field result are of the same order of magnitude. However, in the correlated case, $U \neq 0$, low-temperature enhancement of the electronic specific heat of the exact solution over the mean-field result is observed. This shows that collective excitations are taken into account in the exact solution. The magnetic spin susceptibility was evaluated for parameter values U = 10eV, t = 1eV (figure 3). Also shown for comparison

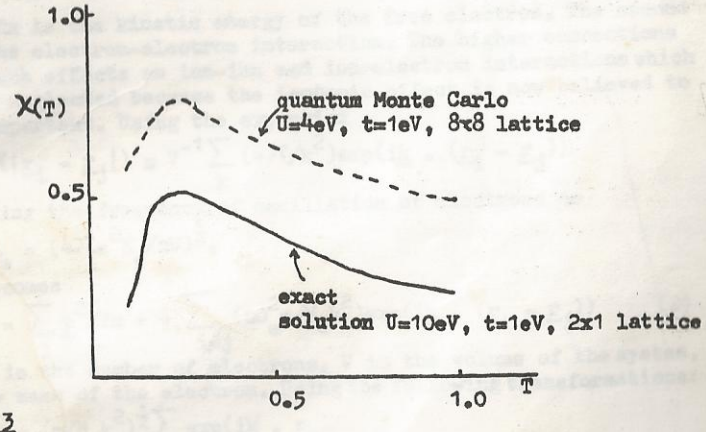


Figure 3

is the magnetic spin susceptibility for an 8 x 8 lattice, obtained by quantum Monte Carlo calculations (White et al, 1989). We see that they are similar in shape and differ by a constant over most of the range. We may conclude from this that the exact solution of the 2 x 1 lattice incorporates the essential features of a larger lattice solution. Further work is in progress.

REFERENCES

L. N. Bulaevskii, V. L. Ginzburg, & A. A. Sobyanin, (1988) Physica, C152, 378
K. A. Chao & K. F. Berggren, (1975) Phys. Rev. Lett., 34, 880
D. M. Ginsberg, (1989) in "Physical properties of high temperature superconductors", (L. M. Ginberg, Ed.), World Scientific
J. B. Goodenough & A. Manthiram, (1988) "Progress in high temperature superconductivity", 5, World Scientific
J. Hubbard, (1963) Proc. Roy. Soc., A276, 238
Y. Muo, N. Kobayashi, & T. Sasaki, (1988) "Proceedings of the Tokai University International Workshop", Tokyo
J. Rossat-Mignod, L. P. Regnault, C. Veltier, P. Burlet, J. Y. Henry, & G. Lapertot, (1991) Physica, B169, 58
J. Thouless, (1961) "The quantum mechanics of many-body systems", Academic Press, New York
S. R. White et al, (1989) Phys. Rev. B, 40, 506
F. C. Zhang & T. M. Rice, (1988) Phys. Rev., B37, 3759