Dynamic Properties of Interacting Electrons.

Lun Tan

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Dynamic properties of interacting electrons

Tan, Lun, Ph.D.
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in

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by

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TO MY PARENTS
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ABSTRACT

The spectral weight functions and the optical conductivity of a highly correlated electronic system described by a simple Hubbard model are studied. The calculations are carried out for a small system, a cubic cluster of eight sites, by means of exact diagonalization using symmetrized basis functions.

The spectral weight functions of a single hole (or electron) placed in an otherwise half-filled band are obtained. The density of states at different interaction strengths, ranging from weak to strong couplings, is studied. We observe the spreading of the spectral weight associated with some single-particle eigenstates over a large range of energies, and the appearance of satellite structure at higher excitation energies. The nature of band narrowing is also discussed.

The frequency dependent (optical) conductivity is studied for the cases of a half-filled band, and for one hole and two hole dopings away from half filling. The interaction strength is varied between the weak- and strong-coupling limits. The formation of a Hubbard gap is observed. Results are related to aspects of the metal-insulator transition in bulk systems.
CHAPTER 1
INTRODUCTION

This dissertation presents the study of two dynamic properties of a highly correlated electronic system: spectral weight function [1] and optical conductivity [2].

In a highly correlated electronic system, such as a 3d transition metal oxide, the valence electrons strongly interact with each other. This kind of system may exhibit some properties, such as long range magnetic order [3], heavy fermion behavior [4,5] and high temperature superconductivity [6,7] which often cannot be understood correctly by conventional local spin density band theory. The reason for the failure of conventional band theory is that the electron-electron interaction is so strong that the approximate picture of one electron moving in an average potential does not hold. Although Landau’s Fermi liquid theory [8] proposed the concept of quasiparticles which may extend the one particle band picture to systems where the interactions are not very weak, a generic question immediately arises: Is there an upper limit to the interaction strength beyond which the quasiparticle picture will fail?

In order to investigate these questions, it is necessary to consider a Hamiltonian which takes into account significant electron-electron interactions. In other words, one has to deal with a many particle Hamiltonian instead of a one particle Hamiltonian. The model Hamiltonian method is widely used to deal with this kind of problems. In this method, the model is obtained by making some approximations to the full Hamiltonian which includes long
range Coulomb interactions, retaining only one or a few terms which describe short range electron-electron interactions. Two typical examples are the Hubbard model [9] and the Anderson model [10]. One then tries to diagonalize the Hamiltonian matrix to get the eigenenergies and eigenstates of the system. Although these model Hamiltonians are algebraically simple, exact solutions are rare and can only be obtained in some special cases [11,12].

Many kinds of approximate techniques have been used in order to get solutions in other than such special cases. For example, there are techniques such as mean-field theory [13], Green function decoupling schemes [14], functional integral formulations [15], and variational approaches [16] which have been used to study the Hubbard model. Frequently, however, uncontrolled approximations in these methods greatly undermine the reliability of the results.

Another approach is to solve the model Hamiltonian exactly on small finite systems (clusters) either by exact diagonalization (or Lanczos algorithm) methods [17] or by quantum Monte Carlo techniques [18]. One then tries to link the results obtained for a small system to the behavior of a bulk system. The problem of such a linkage is of vital importance for this approach. In this dissertation, the finite system approach is adopted. More specially, we diagonalize a one-band Hubbard Hamiltonian on an eight-site simple cubic cluster. The Hubbard model was first proposed by J. Hubbard in 1963 [9] and is described below.

Let $\phi_{\sigma}(r - R_i)$ denote the local basis function (Wannier function, for example) of an electron with spin $\sigma$ on the atom at site $R_i$, $c_{i\sigma}^\dagger$ as the creation operator which creates an electron at site $R_i$ of spin $\sigma$, and $c_{i\sigma}$ as the corre-
sponding annihilation operator. In this basis, only one local wave function or orbital is considered on each site. The Hamiltonian for the electrons in a non-degenerate band can be written in the notation of second quantization as:

\[ H = \sum_{i,j,\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \frac{1}{2} \sum_{i,j,k,l,\sigma,\sigma'} <i\sigma,j\sigma'|\frac{1}{r}|k\sigma,l\sigma'> c_{i\sigma}^\dagger c_{j\sigma'}^\dagger c_{l\sigma} c_{k\sigma'}. \] (1.1)

where

\[ t_{ij} = \int \phi^*(r-R_i)\left[-\frac{\hbar^2}{2m}\nabla^2 + V\right]\phi(r-R_j)dr \] (1.2)

and

\[ <i\sigma,j\sigma'|\frac{1}{r}|k\sigma,l\sigma'> = \left. e^2 \int \phi_{i\sigma}^*(r-R_i)\phi_{j\sigma'}^*(r'-R_j) \frac{1}{r-r'} \phi_{k\sigma}(r-R_k)\phi_{l\sigma'}(r-R_l)drdr' \right| \] (1.3)

The basic approximation made by Hubbard [9], Gutzwiller [16] and many other authors is to retain only the interaction terms with \( i = j = k = l \) and to limit electron hopping to nearest neighbor sites only. These restrictions are generally believed to be appropriate in the description of narrow band materials. With this approximation, the Hamiltonian (1.1) will be simplified to the simple one band Hubbard Hamiltonian below:

\[ H = t \sum_{<i,j>,\sigma} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}. \] (1.4)

In Eqs. (1.1) – (1.4) the \( c_{i\sigma}^\dagger (c_{i\sigma}) \) are the creation (destruction) operators which create (destroy) electrons of spin \( \sigma \) on site \( i \); \( n_{i\sigma}(i) = c_{i\sigma}(i)^\dagger c_{i\sigma}(i) \) is the
number operator for electrons of spin up (down) on site \( i \); \( t \) is the transfer integral, and \( U \) is the electron interaction parameter. The summation in the first term runs over all nearest neighbors, \( i \) and \( j \). It describes electron hopping between nearest neighbor lattice sites \( i \) and \( j \). The second term in the equation describes the interaction between electrons of opposite spin on the same site. It is believed that this model is the simplest one which makes a connection between band-like and atom-like properties in solids, especially for d-band materials such as transition metal oxides and high temperature superconductors.

The specific system which we study is an eight-site simple cubic cluster with lattice sites located at each corner of a cube (Fig. 1). Although there are no monatomic simple cubic crystals in nature, the simple cubic lattice is frequently studied theoretically because it is the simplest three-dimensional geometry.

Numerical studies of this three-dimensional Hubbard system has been reported previously. Kawabata determined the spin of the ground state as a function of \( U/t \) for filling from two to eight electrons [19]. Spin-correlation functions and thermodynamic properties were obtained in Ref. [20]. Much work has also been done on the Hubbard model for two-dimensional systems. A review of some related aspects is given in Ref. [21].

The eigenvalues and eigenstates of the Hamiltonian are generated by exact diagonalization using symmetrized basis functions [17]. In this method, the Hamiltonian matrix is expressed on the basis of occupation numbers.
Fig. 1. The picture of an eight-site simple cubic cluster.
Denote the basis functions as $|n>$, then each one of these functions will be an eigenfunction of the number operator $\hat{n}$

$$\hat{n}|n> = n|n>.$$  \hspace{1cm} (1.5)

The size of the matrix we need to diagonalize in our calculation can be greatly reduced by taking symmetry considerations. First the total spin $S$ and the $z$ component of the spin $S_z$ of the system are good quantum numbers. Therefore the eigenenergies and eigenstates can be calculated in the subspace of fixed $S_z$ (fixed number of spin-up and spin-down electrons). Secondly, by applying spatial symmetry (cubic $O_h$ in our case) operations to reconstruct the basis functions, the Hamiltonian matrix may be further converted into a direct sum of a series of submatrices whose dimensions are much smaller than that of the original matrix. Each submatrix is then diagonalized and the collection the eigenvalues and eigenstates of the submatrices provides a complete spectrum of the eigenvalues and eigenstates of the Hamiltonian.

The discovery of high-$T_c$ superconductivity in copper oxide systems has focused attention on the propagation of holes in an antiferromagnet which are often described in terms of the Hubbard model and its extensions. $La_2CuO_4$ is an insulating antiferromagnet. It becomes a superconductor when electrons are removed through the replacement of a small percentage of trivalent La by divalent Ba or Sr. In order to investigate the propagation of holes (or electrons) in such a system, it is desirable to study the spectral weight function of a single hole (or electron) placed in an otherwise half-filled band described by the Hubbard model.
The study of the spectral weight function by using small clusters goes back to Harris and Lange [22]. They calculated the density of states and spectral weight function analytically for a two-site Hubbard system and showed in their results that in atomic limit with one electron per atom, the spectral weight function has a series of bands separated in energy by $U/t$. Brinkman and Rice [23] calculated the spectral weight function on a simple cubic lattice in the atomic limit of the Hubbard model by means of Nagaoka's path formulation method [12]. They predicted that a substantial amount of band narrowing is caused by the electron-electron interaction, with tails extending out to the full free-particle width. This important prediction needs confirmation based on numerical techniques since the approximations used in their derivation are not well-controlled. Since then, a series of calculations have been made on the $t - J$ model (a list of papers can be found in Ref. [24]) which can be viewed as an approximation to the Hubbard model in the strong $U$ (atomic) limit by imposing the restriction that no two electrons can be on the same site at the same time. The $t - J$ model Hamiltonian has the following form:

$$H_{t-J} = t \sum_{i,j,\sigma} (1 - n_{i-\sigma})c_{i\sigma}^\dagger c_{j\sigma}(1 - n_{j-\sigma}) + J \sum_{i,j} \mathbf{S}_i \cdot \mathbf{S}_j$$

(1.6)

where the first term is the hopping term similar to that of the Hubbard model provided that double occupancy is not allowed. The second term represents the antiferromagnetic Heisenberg spin interaction between electrons on nearest neighbor sites. The quantity $J$ is related to $U$ by $J = 2t^2/U$. This model does not connect in any simple ways to the weak interaction limit ($U \ll t$) of the Hubbard model. The most important reason for us
to study Hubbard model is that it offers a weak interaction limit where we know the quasiparticle description must be valid. Therefore, it is possible to trace the quasiparticle peaks, going from small $U$ to large $U$, based on the principle of continuation. In the exactly half-filled-band limit (zero hole), the $t - J$ model reduces to an antiferromagnetic Heisenberg model. Most of the calculations on $t - J$ model concern on square lattices. An important work [24] gives results for Hubbard model on eight- and ten-site square lattices by exact diagonalization. There is, however, a significant difficulty in interpreting the results for an eight-site square lattice: the spectrum of single-particle states contains only three levels; two of which are nondegenerate and the other one is six-fold degenerate. This high degeneracy is accidental since the maximum degeneracy of single-particle states resulting from the symmetry of a two-dimensional square lattice is two. This leads to an unrealistically large peak in the density of states in the interacting system near the Fermi energy. In contrast, for a cubic cluster, the maximum degeneracy permitted by symmetry of the single-particle levels (Fig. 2) is three, which offers a very natural correspondence with a bulk system.

Freericks and Falicov [25] have pointed out that for a self-contained Hubbard cluster, such as our eight-site cubic cluster, the results with periodic boundary conditions which are more appropriate for the discussion of bulk properties may be obtained by simply multiplying the transfer parameter by 2. That is, if we obtain the results for, say, $U/t = 16$, the corresponding value of $U/t$ for an infinite system is 32. The width of the spectrum shown in Fig. 2 will also be doubled. This renormalization of $t$ can be justified by noticing that the summation over nearest neighbors in the first term of
Eq. (1.4) will just be doubled had we impose periodic boundary conditions instead of open boundary conditions to our system.

Our consideration of a cubic cluster instead of a square lattice means that we are not trying to draw conclusions directly pertaining to high-$T_c$ superconductivity, but rather to address the physical question of how useful it is to describe the electron (hole) propagation by means of single-particle eigenstates for different strengths of the short range interaction. This question is of significant importance to the cubic transition-metal oxides.

Another subject of much recent interest is the metal-insulator transition. Is there a metal-insulator transition in a many-body electronic system as the interaction strength increases? If there is, when does it happen? Two factors may contribute to this transition. As the interaction strength $U/t$ increases, a so called Hubbard gap may eventually appear which leads the system to change from a metallic state to an insulating state. Another factor is electron localization. In a highly correlated system, the short range interaction tends to localize electrons. The electron localization reduces the conductivity and may leads the system to become an insulator even before a substantial energy gap appears. In his classic paper, W. Kohn [26] pointed out that a finite energy gap may not be necessary in defining an insulator. Kohn also showed that the real part of the zero frequency optical conductivity, which is often referred to as the Drude term, may be used as a probe to investigate the metal-insulator transition. For a large system, the integrated weight of the Drude term would vanish for an insulator and be finite for a metal.

Some work has been done on calculating the optical conductivity of the Hubbard model. Much has concerned one- and two-dimensional systems
[27-43]. Exact diagonalization methods (such as Lanczos algorithm) have generally been used. Much less attention has been given to three-dimensional systems. We calculated the optical conductivity of the Hubbard model on an eight-site cubic cluster. Since the wavelengths of infrared and optical phonon are very large compared to the lattice constants of crystals, the wave vector $q$ of a photon emitted or absorbed can generally be neglected, and one considers the conductivity only in the case $q=0$. This is referred to as the optical conductivity.

The rest of the dissertation has been organized as follows: Chapter 2 presents our work on the spectral weight function. Section 2.1 gives the method of calculation; The numerical results are shown in Section 2.3, Section 2.4 contains the conclusions. Calculations of the optical conductivity are discussed in Chapter 3. Section 3.1 is an introduction; section 3.2 presents the calculational procedures; section 3.3 shows the results in detail. Finally in Section 3.4, the conclusions are summarized.

Some sample computer programs are included in the Appendix.
In this chapter, we present calculated results for the spectral weight function on an eight-site simple cubic Hubbard cluster. The calculation is made by exact diagonalization. The results are obtained for a hole placed in an otherwise half-filled band case only. The first section gives the definition of the spectral weight function and derives the formula we used in our calculation. The second section presents and discusses the results obtained for different interaction strengths. We observe the spreading of the spectral weight associated with some single particle eigenstates over a large range of energies, and the appearance of satellite structure at higher excitation energies. The nature of band narrowing will be described. The last section summarizes the results and gives the conclusions of this chapter.

2.1 The Method of Calculation

The spectral weight function is defined as a quantity which is directly proportional to the imaginary part of the Fourier transform of one particle Green’s function. It is a quantity which is associated with the process of adding a particle (electron or hole in our system) to a system. This quantity, denoted by $A_\gamma(\omega)$, describes the probability of a particle being in a single particle state $\gamma$ and having energy $\omega$ when it is added to the system. Here $\gamma$ is an index which identifies a single particle state. It may include wave vector $k$, band index, spin or other quantum numbers.
Let's assume that the system we consider contains $n$ electrons. The exact eigenstates are denoted by $|\alpha, n\rangle$ where $\alpha$ numbers the states and implicitly includes relevant quantities such as total wave vector. $\alpha = g$ corresponds to the ground state. Different states are orthonormal:

$$<\alpha, n|\beta, n> = \delta_{\alpha\beta}$$

(2.1)

According to many body theory, the retarded Green's function [8] of an electronic system can be defined as

$$G_{\text{ret}}(\gamma, t - t') = -i\theta(t - t') < c_\gamma(t) c_\gamma^\dagger(t') + c_\gamma^\dagger(t') c_\gamma(t) >,$$

(2.2)

where $\theta(t - t')$ is a step function. $c_\gamma(t)$ is the annihilation operator defined in the Heisenberg picture:

$$c_\gamma(t) = e^{i(H-\mu N)t}c_\gamma e^{-i(H-\mu N)t},$$

(2.3)

c_\gamma is the annihilation operator in Schröedinger picture which annihilates an electron in state $\gamma$. The underlying single particle states, denoted by $\gamma$, are assumed to be eigenstates of a suitable one-particle Hamiltonian. In the Hubbard model, these states result from a diagonalization of the Hamiltonian in the absence of interactions ($U = 0$). $N$ is the average number of electrons in the system, and $< \cdots >$ denotes a thermal average. For the small systems of interest to us, the average is considered to be restricted to states of a fixed number of particles (canonical ensemble). At $T = 0$, $< \cdots >$ becomes to the ground state expectation value. The quantity $\mu$ is the chemical potential which in general is a function of temperature, and has different values for
finite systems with \( N - 1, N \) and \( N + 1 \) particles [50]. Since the value of \( \mu \) does not change the relative positions of the excitation peaks in spectral weight function (as we will see in Eq. (2.7)), we will set \( \mu \) to the value of the chemical potential of \( N \) electron system for the convenience of our discussion. As we will see later, \( \mu = U/2 \) in the half-filled case \( (N = 8) \) and the hole part and the electron part of the density of states are inversions to each other with respect to \( \omega = 0 \), as a consequence of the electron-hole symmetry. By doing some algebraic manipulations one can get the Fourier transform of the retarded Green’s function:

\[
G_{ret}(\gamma, \omega) = \int_{-\infty}^{+\infty} e^{i\omega(t-t')} G_{ret}(\gamma, t - t') d(t - t')
\]

\[
= \frac{1}{Z_n} \sum_a e^{-\beta E_a} \left( \sum_b \frac{|<a, n|c_{\gamma}|b, n+1>|^2}{\omega + E_a - E_b + \mu + i\eta} - \sum_d \frac{|<a, n|c_{\gamma}^\dagger|d, n-1>|^2}{\omega + E_d - E_a + \mu - i\eta} \right).
\] (2.4)

In this expression, \( a \) denotes the states of a \( n \)-particle system. States of \( (n - 1) \) and \( (n + 1) \)-particle systems are denoted by \( b \) and \( d \), respectively. \( \eta \) is a small positive number. \( \beta = (k_B T)^{-1} \) where \( T \) is temperature and \( k_B \) the Boltzmann constant. \( Z_n \) is the partition function:

\[
Z_n = \sum_a e^{-\beta E_a}.
\] (2.5)

The spectral weight function can then be obtained from the following relation:

\[
A_{\gamma}(\omega) = -2 Im G_{ret}(\gamma, \omega)
\] (2.6)
Using the following identity for the inverse of a complex number with a small imaginary part

\[ \frac{1}{\omega + E + i\eta} = P \frac{1}{\omega + E} - i\pi \delta(\omega + E) \]

as \( \eta \to 0 \), we can get the following result from Eq. (2.4) and (2.6):

\[
A_\gamma(\omega) = \frac{1}{\mathcal{Z}_n} \sum_a e^{-\beta E_a} \left[ \sum_b | < a, n|c_\gamma|b, n + 1 > |^2 \delta(\omega + E_a - E_b - \mu) \\
+ \sum_d | < a, n|c_\gamma^\dagger|d, n - 1 > |^2 \delta(\omega + E_d - E_a - \mu) \right] 
\]  

(2.7)

As we can see, \( A_\gamma(\omega) \) is the superposition of a series of \( \delta \) functions which are located at the corresponding excitation energies. This argument also verifies the physical meaning of the spectral weight function: It is the probability of an electron having quantum number \( \gamma \) and energy \( \omega \). We consider these excitations as quasiparticles. In order for the lifetime of the excitations to be long enough so that the quasiparticle description is valid, the \( \delta \) function peaks have to be sharp. Interactions broaden and shift the peak and produce an incoherent background. For bulk systems, the sum in Eq. (2.7) runs over a continuous distribution of states and therefore gives a finite result. For a small system, one should keep \( \eta \) as a small but finite number in order to get finite results and at the same time show clearly the structure.

In a bulk system, there is no essential difference between the states of \((n-1), n, \) and \((n+1)\) particles. Eq. (2.7) can be simplified to

\[
A_\gamma(\omega) = \frac{2\pi}{\mathcal{Z}} \sum_a \left[ \sum_b | < a|c_\gamma|b > |^2(e^{-\beta E_a} + e^{-\beta E_b}) \times \delta(\omega + E_a - E_b) \right] 
\]  

(2.8)
This is a standard result. It, however, can not be applied to finite systems since, for a finite system, the states of \( n \) and \( (n \pm 1) \) systems are distinguishable. We use Eq. (2.4) in our calculation. Several properties of \( A_\gamma(\omega) \) can be obtained:

1. Using the fermion anticommutator relation:

\[
\lim_{t \to t'} (c_\gamma(t)c_\gamma(t') + c_\gamma(t')c_\gamma(t)) = 1,
\]

one can derive the "sum rule" for \( A_\gamma(\omega) \):

\[
\frac{1}{2\pi} \int_{-\infty}^{+\infty} A_\gamma(\omega)d\omega = 1,
\]

This can be used to check on numerical calculations. To apply this relation to an \( n \)-particle system, one has to know the contributions from both \((n - 1)\)- and \((n + 1)\)- particle states (see Eq. (2.4). In the present problem it is often convenient to consider only the contribution from one set of particle states.

For a single, half filled band for which the number of single-particle states is equal to the number of sites \( N \) (times a factor of 2 for spin), we integrate over only one term of the two in Eq. (2.7), and then sum over states of a single spin only to obtain

\[
\frac{1}{2\pi} \sum_\gamma \int A_\gamma^{(h)}(\omega)d\omega = \frac{1}{4}N.
\]

The superscript \( h \) (holes) implies that only the second term of Eq. (2.7) has been considered.
2. If we sum $A_\gamma(\omega)$ over $\gamma$, we obtain a single particle distribution over energies, which is, by definition, the density of states:

$$n(\omega) = \frac{1}{2\pi} \sum_\gamma A_\gamma(\omega), \quad (2.12)$$

3. In this dissertation we calculate the spectral weight function in the half-filled case, that is, $n = 8$. The energy spectrum in simple cubic geometry possesses the property of electron-hole symmetry, which states that for two systems with total number of electrons equal to $n$ and $n'$, respectively, if $n' = 2N - n$ where $N$ is the number of sites, their eigenvalues have the following relation:

$$E_{n'} = E_n + (N - n)U, \quad (2.13)$$

and have the same eigenfunctions. Thus, the energies of corresponding states of 7 and 9 electron system are related by:

$$E_9 = E_7 + U. \quad (2.14)$$

Because of this symmetry, only the eigenstates and eigenenergies of $n - 1 = 7$ need to be calculated. Those for $n + 1 = 9$ can be obtained by simply adding a constant $U$ to the eigenenergies. The chemical potential $\mu = (E_g(n + 1) - E_g(n - 1))/2$ thus have the value $U/2$ in this case. This symmetry also guarantees that the spectral weight function of a half-filled system is symmetric with respect to the zero energy ($\omega = 0$) axis and is the same for positive and negative values of $U$ [44]. Our calculation is for positive $U$ only.
A further simplification can be made by calculating $A_\gamma(\omega)$ at zero temperature, or in other words, the ground state spectral weight function. In this case, Eq. (2.4) becomes

\[
G_{\text{ret}}(\gamma, \omega) = \left[ \sum_b \frac{|<g, n|c_\gamma|b, n + 1>|^2}{\omega + E_g - E_b + \mu + i\eta} \right. \\
+ \sum_d \frac{|<g, n|c_\gamma^d|d, n - 1>|^2}{\omega + E_d - E_g - \mu + i\eta} \right].
\] (2.15)

Our calculation is based on this expression.

We would like to make a general remark on the effect of selection rules on the spectral weight function. Consider the hole excitation part which corresponds to the second term in Eq. (2.15). We start initially with the ground state of half-filled case, $|\phi_0> = |g, n>$, which has definite total spin, $z$ component of spin and space symmetry. We then annihilate a (spin-up) electron with single particle state index $\gamma$. The resultant state $c_\gamma|\phi_0>$ must have definite space symmetry and also satisfy selection $|S' - S| = 1/2$ and $S_z' = S_z - 1/2$. The overlap of this state with different eigenstates of the one-hole systems determines the weight and shape of the spectral weight function. But the contribution is nonzero only for those states which have the proper spin and space symmetry.

In our computer program, the the ground state energy and wavefunction of the $N$-particle system are first generated and stored in memory ($N = 8$). Since the system which we deal with here had been studied before [20], we can use some of the results obtained from the previous work. Then the eigenenergies and eigenstates of the $(N-1)$-particle system are generated and the matrix elements $<g, n|c_\gamma|d, n - 1>$ as well as the sum in Eq. (2.15) are
calculated to get the retarded Green's function \( G_{\text{ret}}(\gamma, \omega) \). The eigenenergies and eigenstates associated with the \((N + 1)\)-particle system can easily be obtained by means of Eq. (2.14) for \( N = 8 \). Not all the matrix elements need to be considered. The probability of transitions from the ground state of \( N \)-particle system to the high energy states of \((N \pm 1)\)-systems (compared to their own ground state) is very small and the corresponding matrix elements can be neglected. We therefore set a cut-off energy \( \text{ELIM}_n \) for the \( n \)-particle system \((n = N \pm 1)\) above which the matrix elements are neglected. This energy is usually set in the way that its difference from the ground state energy of the \( n \)-particle system is about the bandwidth of the noninteracting system \((\text{ELIM}_n - E_g^{(n)} \sim 6)\). \( E_g^{(n)} \) is the ground state energy of \( n \)-particle system which is known from the previous work. The results can also be checked by means of the sum rule Eq. (2.10) or (2.11).

The spectral weight function and the density of states are then be calculated by means of Eq. (2.6) and (2.12).

### 2.2 The Numerical Results

The numerical results for the spectral weight function and density of states for an eight-site simple cubic cluster at half-filled case with open boundary conditions are reported below. For periodic boundary conditions, the results are the same except for a change of \( t \) to \( 2t \). A wide range of correlation strengths \( U/t \) and all allowed wave vectors have been covered in our calculation. To start our discussion, let's first look at the results for \( U = 0 \). In this situation, the Hubbard Hamiltonian (1.4) can be solved exactly analytically. The single particle eigenstates and eigenenergies are shown in
Figure 2. The energy levels are at $E = -3t, -t, t$ and $3t$. with degeneracy (not including spin) equal to 1, 3, 3 and 1, respectively. Let's label these four levels as 1, 2, 3 and 4. In a periodic model, level (1) is associated with point $R$ in the Brillouin zone, $\mathbf{k} = (\pi/a, \pi/a, \pi/a)$; level (2) is associated with point $M$, $\mathbf{k} = (\pi/a, \pi/a, 0)$; level (3) is associated with point $X$, $\mathbf{k} = (\pi/a, 0, 0)$; and level (4) is associated with point $\Gamma$, the origin. In half-filled case, level (1) and (2) are fully filled with electrons, level (3) and (4) are empty for the ground state. As expected, the calculated ground state density of states at $U = 0$ consists of four peaks centered at $E = -3t, -t, t$ and $3t$. The $E > 0$ portion corresponds to states in which an extra electron has been added to the system, which will increase the energy of the system by $E$. On the other hand, the $E < 0$ portion corresponds to states from which an electron has been removed or a hole has been added. In this case, energy $E$ has to be added to the system. We designate $|E|$ as the excitation energy. In the photoemission literature, $|E|$ is usually called the binding energy. Note that the density of states is symmetric with respect to $\omega = 0$. This always holds for simple cubic cluster due to the electron-hole symmetry.

We would like to discuss our results in the increase order of $U$. First let us look at the weak coupling region. Fig. 3 shows the density of states for $U=1$. The following observation has been made:

1. The positions of the large peaks associated with triply degenerate states remain almost unchanged relative to those in the noninteracting system. The separation between them does not increase when $U$ is still small. This shows that the formation of the Hubbard gap does not begin at this point.
Fig. 2. Illustration of the single-particle levels in the cube. The energies are indicated on the left and the spatial degeneracies in parentheses on the right. Levels are numbered in order of increasing energy.
Fig. 3. Density of states for $U = 1$. Both holes and electron contributions are shown. The numbers in parentheses indicate the single-particle level associated with the peak. The curves are computed using a width parameter $\eta = 0.05$. All energies are ratios with respect to $t$. 
2. The peaks associated with level (1) and (4), namely the two non-degenerate states at $U = 0$ split. But the center of gravity of each split pair remains the same as that of the relevant state in the noninteracting system.

3. The area under the peaks shown, satisfies the sum rule, Eq. (2.10). Thus, apart from the splitting mentioned above, many-body effects are not significant. The changes produced in the system by the addition or removal of a single particle are well described in terms of occupation of single-particle states. Apart from the splitting, Fig. 3 reproduces the results of a noninteracting system.

4. The splitting is a many body effect. It can be understood as follows: Consider the hole portion. At $U = 0$, the state of $(n - 1)$-particle system with one deep hole in level (1) is degenerate with the state of having two holes in level (2) and one excited electron in level (3). When $U = 0$, the latter state is not accessible from the ground state of half-filled system by excitation of a single hole. Therefore, it has no contribution to the spectral weight function and the density of states shows only one single peak at $E = -3t$. When $U \neq 0$, the degeneracy of the two $(n - 1)$-particle states is lifted by interaction. Both states are accessible from the $n$-particle ground state. The two states are mixed with approximately equal amplitude and the amount of the splitting between them is proportional to $U$. This results in the splitting we have seen in Fig. 3 where peaks $1U$ and $4L$ correspond to the original quasiparticle excitations pertained from $U = 0$, while peaks $1L$ and $4U$ belong to the multi-channel excitations which show up as $U$ turns on and form the (presumably) incoherent background.
The different behavior of the peaks associated with level (1) and level (2) in the hole band can be attributed to the fact that the former describes a state at the bottom of the single-particle band and the latter a state at the Fermi energy. This phenomena has been observed in many other systems [49] and can also be described by Fermi liquid theory. It is a general feature of the interacting electron system. The quasiparticles close to the Fermi surface are expected to be sharp, while peaks further away from the Fermi surface broaden due to the greater probability of decay into multiple particle-hole channels.

5. It is observed that the position of the quasi-particle peaks close to the Fermi energy are independent of $U$ for small $U$. More precisely put, if we expand the position of the peaks as a power series of $U$, the first order term vanishes. This can be proved as follows: For the half-filled system with all sites equivalent, there is one electron per site on average. Each site can hold two electrons, one spin up and one spin down. Hence, the average value of $\langle n_{i\uparrow}n_{i\downarrow} \rangle$ is $1/4$. When one electron is added or removed, this average becomes to $\frac{1}{2}(\frac{1}{2} \pm \frac{1}{N})$. Therefore, the ground state energy for the $N$-particle system is:

$$E_g(N) = E_0(N) + NU/4,$$

and for $(N \pm 1)$-particle system

$$E_g(N \pm 1) = E_0(N \pm 1) + (N/4 \pm 1/2)U + O(U^2).$$
The corrections are of order $U^2$ and higher. Here $E_0$ is the energy of the non-interacting system. From Eq.(2.15) we see that the peaks on the hole side occur when

$$E = E_g(N) - E_d(N - 1) - \mu, \quad (2.17)$$

where $d$ is some eigenstate of the $(N - 1)$-particle system. Since the chemical potential $\mu = U/2$ for a half-filled system with electron-hole symmetry, we see that

$$E = E_0(N) - E_d^{(0)}(N - 1) + O(U^2), \quad (2.18)$$

where the first order term of $U$ vanishes and $E_d^{(0)}$ is the energy of a state $d$ of a noninteracting system with $N - 1$ electrons. This is the reason why the positions of the two peaks corresponding to the triply degenerate levels remain almost the same in Fig. 3 ($U = 1$) as that for the noninteracting system ($U = 0$). This argument breaks down if the ground state of $N$ or $N \pm 1$ particle system is degenerate when $U=0$ and non-degenerate when $U \neq 0$. In this situation, a first order term in $U$ appears in the expression for the peak position as we have seen in the splitting shown in Fig. 3.

As $U$ increases, the system enters the intermediate coupling region. We roughly define this region as $3t < U < 18t$ for our cubic cluster. This is the most interesting region from the point of application to real materials – 3d transition metal magnet, oxides, and cuprate superconductors. In this region the local moments form and antiferromagnetic correlations develop in a half-filled system [52]. Fig. 4 shows the density of states at $U = 4$. As $U$ increases, we see that: 1. While the major peaks remain, the magnitude of peaks (2) and (3) referring to the highest hole and lowest electron level have
Fig. 4. Density of states for $U = 4$, computed with a width parameter $\eta = 0.05$. 
been reduced, so do the peaks (1U) and (4L). In contrast, the magnitude of peaks (1L) and (4U) have increased.

2. Some additional structures appear: processes once prohibited in non-interacting system, such as hole propagation in level (3) and (4), or electron propagation in level (1) and (2), show some contributions.

3. The separation between (2) and (3) begins to increase, from 2t in Fig. 3 to 2.5t in Fig. 4. This suggests the beginning of the formation of a gap associated with anti-ferromagnetism (as in the work of Kampf and Schrieffer [45]). This gap will eventually develop into the so-called Hubbard gap as $U$ increases. We have known from previous spin-correlation function calculation [20] that the ground state of the half-filled system is antiferromagnetic for intermediate and large values of $U$. But it is difficult to determine the exact value of $U$ for which this gap shows up in the corresponding bulk systems due to the finite size of our system.

When $U$ increases to 8, the density of states, as shown in Fig. 5, shows that the separation between the peaks labeled (2) and (3) at the top of the lower band and the bottom of the top band has reached 5.1t. The electron and hole portions (upper and lower Hubbard bands) are clearly separated. We have a distinct Hubbard gap at this point. The additional structure becomes obvious. As a result, the lower and upper Hubbard bands are broadening, each developing structure at higher excitation energies, indicating that an incoherent background is developed. For example, there are peaks associated with single particle levels (3) and (4) in the hole band, while peaks associated with levels (1) and (2) appear in electron band. These peaks are not allowed in the noninteracting limit.
Fig. 5. Density of states for $U = 8$, computed with $\eta = 0.05$. 
The appearance of this additional structure can be explained as following: consider the extra peaks on the hole side. As $U$ increases, the contribution to the total energy from the on-site interaction increases. Electrons tend to avoid double-occupancy in the ground state of $N$-electron system by partially filling level (3) or (4) instead of doubly occupying level (1) and (2). This leaves two (or more) holes in level (1) or (2) and the same number of electrons in level (3) and (4). When an operator $c_\gamma^\dagger$ removes an electron from level (3), for example, it may create a peak associated with level (3) in the spectral weight function and produce an $(N - 1)$-particle state which contains a hole and an electron-hole pair. Those peaks which belong to the additional structure will appear at excitation energies which are larger by the amount required to create an electron-hole pair.

At $U = 8$, the integrated weight under the additional structure is just $1/3$ of that under original structure, which refers to the structure associated with the levels (1) and (2) for holes and (3) and (4) for electrons. As $U$ increases further, the integrated weight under additional structure will increase. Eventually, in the large $U$ limit, it becomes the same as that of the original structure.

The Hubbard gap increases as the interaction strength increases further. At this time, we drop the chemical potential $\mu$ (set $\mu = 0$ in Eq. (2.15)) and show only the hole part of the density of states. The electron part remains identical in appearance. The peaks appear exactly at the energies which correspond to the energy difference between the $N$-electron ground state and the various states of the $(N - 1)$-electron system.
Fig. 6 shows the hole part of the density of state at $U=16$ with $\mu$ set to zero. The peaks at positive energies on this scale result from levels near the bottom of the lowest manifold of states of the $(N - 1)$-particle system. When the interaction parameter $U$ is sufficiently large, all the states of the $N$-particle system are higher in energy than some of the states of the $(N - 1)$-particle system (the $N$-particle system could lower its energy by emission of an electron). We can identify two distinct regions in the graph. One is the upper portion ($E > -0.5$) which contains large peaks associated with level (1) and (2). In the negative energy part region in which the density of states is low, there is another region containing the "forbidden" level (3) and (4). These two regions are separated by a pseudo-gap. Let's study the upper portion first. If we plot the spectral weight functions associated with level (1) and (2) separately, as shown in Fig. 7 and 8, we find that there are two peaks associated with level (1). The larger was evolved from the lower of the two split peaks of nearly equal strength for $U = 1$ (Fig. 3). The upper, which is usually considered to be the quasi-particle peak, has much less weight. On the other hand, although the original quasi-particle peak remains for level (2), much weight has been distributed over additional peaks which occur for a wide range of energies. The weight left for the original quasi-particle peak is only 1/4 of that in the case of $U = 1$. This would correspond to substantial broadening of level (2) in a bulk system.

The lower portion is mainly contributed from the "forbidden" states of level (3) and (4). (However, peaks of level (2) and (3) appear in both regions). It is separated from the upper portion by a pseudo-gap which results from the small matrix elements associated with level (2) and (3). At $U = 16$, the
Fig. 6. Density of states for $U = 16$, computed with $\eta = 0.05$. Only the energy region corresponding to hole states is shown, and the chemical potential has been set to zero.
Fig. 7. Spectral weight function for level 2 at $U = 16$, computed with $\eta = 0.05$. Since this level is threefold degenerate, the vertical scale must be multiplied by 3 to obtain the contribution to the density of states. The factor of $(2\pi)^{-1}$ in Eq. (2.10) has been absorbed into $A$. 
Fig. 8. Spectral weight function for level 1 at $U = 16$, computed with $\eta = 0.05$. 
upper portion still outweighs the lower portion substantially. With increasing $U$, the two portions tend to become of equal weight and the density of states is symmetric about $E = 0$, as shown in Figs. 9, 10 and 11 for the density of states for $U = 32, 100$ and 1000. At large $U$ limit, the Hubbard model is equivalent to the $t - J$ model. This symmetry in the density of states can be proved by applying a canonical transformation, $c_{i\sigma} = (-1)^{m+n}c_{i\sigma}$ to Eq. (2.6) [51].

We believe that many physical transition metal antiferromagnets, probably including those such as (pure) $La_2CuO_4$ which are closely related to high temperature superconductors, are likely to have properties similar to those shown in our Hubbard model calculations in the intermediate range of $U/t$ values. We have sampled this range for $U/t = 4, 8$ and 16. In this range, essential features of the level structure calculated for small $U$ persist, but there will be significant broadening. The density of states is actually broader than found for small $U$, in that satellite contributions from forbidden levels appear at higher excitation energies.

Next, we consider strong $U$ limit. Fig. 9, 10 and 11 show the hole portion of the density of states for $U/t = 32, 100$ and 1000, respectively. As $U$ increases, the satellite region strengthens and the band shifts slightly higher in energy, so that at $U = 1000$ it is very nearly symmetric about $E = 0$, as mentioned above. All the states in this limit have almost the same probability to be occupied, no matter how far above or below the Fermi energy. For an infinite system in this limit, it is expected that there is no discontinuity in the distribution function as required by the Fermi-liquid theory. The Fermi-liquid picture fails. The energy scale is nearly rigid in this
Fig. 9. Density of states for $U = 32$, computed with $\eta = 0.05$. Hole portion only.
Fig. 10. Density of states for $U = 100$, computed with $\eta = 0.05$. Hole portion only.
Fig. 11. Density of states for $U = 1000$, computed with $\eta = 0.05$. Hole portion only.
range of $U$. The ground state energy of the $N$-electron system has a value of order of $(-)t^2/U$ and hence approaches zero slowly as $U$ increases, while the ground manifold of the $(N-1)$-electron system stretches from (roughly) $-3t$ to $3t$. The two symmetric portions are separated by a pseudo-gap located around zero excitation energy. The gap is not a real one since there are a few small peaks associated with levels (2) and (3) which appear inside it. So the density of states is greatly reduced rather than being actually zero. Examination of the energy spectrum of $(N-1)$-electron system reveals that there are some states of the correct symmetry to produce peaks inside the gap. But the matrix elements connecting those states with the ground state of the $N$-electron system are very small.

As argued by Brinkman and Rice [23], the electron-electron interaction leads to substantial narrowing of the quasiparticle band. To investigate this argument on the basis of numerical calculations, one would like to discuss the changes of bandwidth with respect to the interaction strength $U$. Before starting the discussion, one should aware that the general picture given for bulk systems at intermediate and large $U$ by approximate, analytic calculations [53-56] is that there are quasiparticle peaks at the bottom of an incoherent hole band. The weight of the quasiparticle peaks is small for large $U$, vanishing as $U \to \infty$. The energy range of the quasiparticles is fairly small (narrow hole band), but the incoherent part spans a much large range. Based on this picture, we define two different bandwidth. one is width of the quasiparticle band which consists of only the quasiparticle peaks, such as peak 2 and 1U. We denote this bandwidth by $W$. The second is the width of the overall band which is composed of all the major peaks, including both
the quasiparticle peaks and the incoherent background. The energy range spans by this band is denoted by $\Delta$, which is the overall bandwidth. We would like to study the behavior of these two bandwidth as a function of $U$.

There is an additional technical complication while we study the overall bandwidth $\Delta$. When $U > 39.5$, the ground state of the $(N - 1)$-particle system is fully spin aligned for the special geometry of our system. At $U = 1000$, not only the ground state, but the lowest 13 states have $S > 1/2$. Since the ground state of the $N$ particle system is always a singlet $S = 0$, and the operator $c_7$ has spin $1/2$, the transitions between the $N$-particle ground state and the lowest 13 states of the $(N - 1)$-particle system is forbidden by the spin conservation law. As the 13 states span a range over $0.36t$, and the highest state of $S = 1/2$ is below the top of the lowest manifold by $0.39t$, the energy range of the states which can be reached from the ground state of the $N$-particle system is $5.25t$. This corresponds to a 12.5% overall band narrowing for the lowest manifold (total width=6$t$).

The modest narrowing of $\Delta$ is caused by the presence of states unreachable from the singlet ground state of the $N$-particle system by a single particle transition. However, this doesn’t mean that there is no overall band narrowing until the ground state of the $(N - 1)$-particle system becomes ferromagnetic as $U$ increases. In fact, when $U = 32$, the overall band width is $5.4t$, a 10% reduction compared to the non-interacting system. The ground state of the $(N - 1)$-electron system has antiferromagnetic correlations [20] at this $U$, and both $N$ and $(N - 1)$-electron systems have nearly the maximum possible average local moment. In this case, the highest peak of the hole part is still associated with level (2), and is located exactly at the place
corresponding to the energy difference between ground states of the $N$ and $(N - 1)$-particle systems. However, the area under the peak is only $1/6$ of that in the non-interacting system. This is a significant remnant of the quasiparticle picture of the noninteracting system but now the subsidiary peaks are important and have almost three times the integrated area of the highest peak of the hole part. We interpret this as indicating large broadening in bulk system. As $U$ increases, the area under the highest peak continues to decrease.

We have seen from our analysis that the above overall band includes all the multipeak structures exhibited in the spectral weight function. For an actual system, however, only quasiparticles with low excitation energy are relevant to most of the experiments. We therefore would like to investigate the band of quasiparticles which consists of only the quasiparticle peaks with low excitation energy. Its bandwidth $W$ is then the largest energy difference of these quasiparticles. To see more clearly how these peaks behaves, we show in Fig. 12 the motion of the positions of the principle peaks in the hole portion of the density of states on energy scale used above for large $U$ (with $\mu = 0$) as $U$ increases. Some peaks are not present at small $U$. We show them only for larger $U$. The first observation is that the energies increase monotonically with $U$, as is expected. Note that the peaks labeled (2), (1U) and (3) at the top of the overall band are the quasiparticle peaks associated with coherent excitations. They form the band of quasiparticles. As $U$ increases, the bandwidth $W$ changes dramatically. Table 1. shows the bandwidth of quasiparticles for different $U$. We see a substantial band narrowing at strong $U$ limit and consequently, a large effective mass enhancement. The ordering
Fig. 12. Energies of principal peaks in the hole density of states as functions of $U$. 
<table>
<thead>
<tr>
<th>$U$</th>
<th>$W$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0000</td>
<td>2.0</td>
</tr>
<tr>
<td>4.0000</td>
<td>1.9</td>
</tr>
<tr>
<td>10.000</td>
<td>0.4</td>
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<tr>
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<td>0.2</td>
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<tr>
<td>1000.0</td>
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</table>
of the peaks within the band also changes. At $U = 1000$, the bandwidth is only about 10% of the occupied non-interacting band. The upper most peak is the one associated with $1U$ in Fig. 3 where $U = 1$ and the level (2) peak is the highest. This can be explained as the hole levels reordering. There is change in the shape of the hole band in comparison with a more weakly interacting system. The lowest energy hole state is now at $k = (1,1,1)$.

Fig. 12 should be considered together with Fig. 13, which shows the areas under some of the major peaks relating to hole levels. The areas have been normalized according to Eq. (2.10) so that in the non-interacting system, the integrated density of states for a level is 1. (Each level contains one electron of each spin. The spatial degeneracy of 3 associated with level (2) is not included.) In the small $U$ limit, we only have contributions from level (2) and (1), with latter being split into two peaks, as described earlier. In the large $U$ limit, the integrated weight of each level was found to be about $1/2$. (Roughly, all non-interacting levels could be occupied with equal probability, $1/2$ electron or hole of a given spin in each non-interacting state). As we can see from Fig. 13, the weight of the quasiparticle peaks (such as peak 2 and 1U) decrease as the interaction $U$ increases. Consequently, it is difficult to identify these quasiparticle peaks when $U$ is large. Also, in our approach, some quasiparticle peaks may be suppressed by the special geometry we adopted for our system. As we have seen, there is no quasiparticle peak corresponding to level 4 in the hole part of our results. All of these will undermine the reliability of our discussion. Most of the weight is shifted to the peaks consisting of the incoherent background. This is consistent with the picture described by the approximate, analytic methods for bulk
Fig. 13. Areas (dimensionless) under some of the principal peaks in the hole portion of the band (integrated density of states) as functions of $U$. 
systems. Since each level has about the same integrated weight for large $U$, the discontinuity in the occupation number, which exists for weak $U$ limit, will disappear as $U$ become large. This, we believe, suggests that the quasiparticle picture breaks down in strong $U$ limit.

Dagotto and collaborators [24] calculated the spectral weight function for 8- and 10-site Hubbard clusters representing a square lattice with periodic boundary conditions. They considered the interaction strength up to $U = 40$. The different geometries of their systems and the system we considered imply that the energies and the degeneracies of the single particle states of the two kinds of systems are different. However we obtain the same general picture of the variation of the density of states with $U$ as in their work. When $U$ is small, quasiparticles are well defined, and their energies are close to the energies of single particle states. As $U$ increases, additional peaks are found at energies removed from the main peak of the spectral weight function, indicating broadening in the bulk limit. A gap between the hole portion and the electron portion of the density of states begins to build up. At large $U$, each portion is divided by a pseudo-gap centered around zero excitation energy and a substantial narrowing of the bandwidth of quasiparticles is found. There is also indication of a pseudo-gap in Dagotto's work. We believe this general picture is characteristic of the Hubbard model and does not depend on the specific geometry (except for the consequences of hole-electron symmetry, which is found only in bipartite structures).
2.3 Conclusions

In this section, we have reported the results of a calculation of the spectral weight function and density of states for an eight-site simple cubic Hubbard cluster under open boundary conditions as the interaction strength $U/t$ ranges from 0 to 1000. The results present a picture of the behavior of quasiparticles at different interaction strength $U/t$. This behavior is described by the spectral weight function.

The picture we found is this: For weak interactions, the peaks in the spectral weight function remain close to the energies of the eigenstates of the noninteracting system. Those near the Fermi energy are sharp. This is a good indication of the validity of the quasiparticle picture used in Fermi liquid theory. For the states far away from the Fermi energy, if the excitation energy is large enough so that an excited electron or hole may have enough energy to create an additional electron-hole pair, the peak splits. This would correspond in a large system to broadening of the peaks for high excitation energies.

As $U$ increases, additional peaks show up for the states near the Fermi energy (in the noninteracting system). The “original” peaks remain for all values of $U$, but their weight decreases as $U$ increases. More and more weight is shifted to the other peaks. The spectral weight associated with eigenstates at the top of the band (in the case of an extra electron) or at the bottom of the band (for a hole) remain concentrated in a small energy range. Satellite peaks emerge at higher excitation energies. These peaks are mostly, but not exclusively associated with the propagation in levels not accessible in
the noninteracting system, such as hole excitation in the highest level and electron excitation in the lowest level of the system. There is a pseudo-gap between main and satellite regions.

In the strong interacting limit, the satellite peaks gain more weight, finally to become equally weighted as the main band. We cannot identify a quasiparticle unambiguously. The hole and electron portions are (separately) symmetric, each consisting of two parts separated by a pseudo-gap region of low density of states.

There is a modest overall band narrowing as $U$ goes from the weak to the strong interaction limit. In our case, this amounts only to a factor of $1/8$. (The band width at $U = 1000$ is $7/8$ of that at $U = 0$). At extremely large $U$, this band narrowing can be attributed to the operation of Nagaoka’s theorem [12]: the low-lying states of $(N - 1)$-electron system have $S > 1/2$. However, some overall band narrowing also exists in the region where Nagaoka’s theorem does not apply. Most of the overall band width is probably due to incoherent excitations. There is a small region around the top of the hole portion of the density of states where quasiparticle peaks are found. The width in energy of the range of quasiparticle peaks does show substantial narrowing with increasing $U$.

Our results suggest that for realistic electron interaction strengths in transition-metal oxide systems and high-temperature superconductors, the basic band structure picture is robust and will be qualitatively satisfactory and useful for the interpretation of many experiments, such as those involving photoemission. The most important exception is that there will be a Hubbard gap if the interaction is strong enough but the band structure will
not be greatly disrupted except near the Fermi energy. We think this is consistent with experiments on transition-metal oxides [46]. Second, satellite structure in the density of states should be found at higher excitation energy if the interactions are strong enough, even in those cases where a one-orbital model may be adequate.
CHAPTER 3
THE OPTICAL ELECTRIC CONDUCTIVITY

In this chapter, we discuss the calculation of the frequency-dependent optical conductivity on the eight-site simple Hubbard cluster and the results obtained. Section 3.1 gives an introduction and background of the problem. Section 3.2 contains a description of the method we used to do the calculation. The results are described for the half-filled band, as for small hole-dopings away from half filling and are presented in section 3.3. The formation of a Hubbard gap is observed. The results are related to the metal-insulator transition in bulk systems. Section 3.4 presents the conclusions of this chapter.

3.1 Introduction

In general, when an external electric field

\[ E(r,t) = E_0 e^{(iq\cdot r - \omega t)} \]  

(3.1)

is applied to an electronic system, the electric conductivity \( \sigma \) describes the linear response of the system and is a function of the wave vector \( q \) and the frequency \( \omega \). According to the linear response theory, the conductivity of an infinite electronic system can be calculated in principle from the so called "Kubo formula" provided the exact energies and wave functions are known [8,47]. Obviously this is not the case for a highly correlated system. For a highly correlated system, we can only calculate the conductivity numerically.
for a small finite system. In this situation the Kubo formula cannot be applied directly. A different definition of the conductivity is derived which reduces to the Kubo formula as the size of the finite system goes to infinity [39]. We will deal with this in detail in Section 3.2.

As mentioned in Chapter 1, we only want to calculate the optical conductivity \( q = 0 \). In general, one would like to investigate the conductivity \( \sigma \) as a function of band filling and interaction strength \( U \). If dissipative processes are ignored, the real part of \( \sigma \) can be expressed as:

\[
\text{Re} \sigma(\omega) = D \delta(\omega) + \sigma_{\text{reg}}(\omega),
\]

where the first term corresponds to the possibility of free acceleration in a static field \( (\omega \approx 0) \). \( D \) is the so called "Drude weight". \( \sigma_{\text{reg}} \) is the regular part of conductivity which vanishes in a finite system as \( \omega \to 0 \). We can further divide this regular part into two portions: one for intermediate energy \( (\omega \approx t, \text{where } t \text{ is the hopping integral}) \) and another for high energy \( (\omega \approx U) \) in which transitions occur across the Hubbard gap. As mentioned in Chapter 1, Kohn [26] showed that, for a large system, Drude weight \( D \) would vanish for an insulator and would take a finite value

\[
D = \pi e^2 n / m^* \tag{3.3}
\]

for a metal. Here \( n \) is the number of carriers per unit volume, and \( m^* \) is the optical effective mass.

In the Hubbard model for a large system with a half filled band, \( D \) is expected to be zero at least for sufficiently large positive \( U \), and in a one-dimensional system, it is zero for all \( U > 0 \). \( D \) is not zero for other band
fillings. In the case of finite systems, the value of $D$ depends on the boundary conditions imposed on the system. If open boundary conditions are imposed, $D$ is always zero since free acceleration in a static field is not possible. With periodic boundary conditions, the situation becomes quite complicated. In a one-dimensional periodic system with a half-filled band, one finds that $D < 0$ if the ring has $4n$ sites, and $D > 0$ if the number of sites is $4n + 2$ [41]. However, $|D|$ decays rapidly with the size of the ring [40].

In the case of non-half filled band for which $D$ is not zero for a large system, the non-zero $D$ obtained for a finite system with periodic boundary conditions is meaningful. It describes free acceleration. Under open boundary conditions, $D$ is, strictly speaking, zero. In this case there is, however, a peak called the "Drude precursor" in the optical conductivity at low frequency from which the Drude weight $D$ can be extracted by integrating over this peak [39]. The value of $D$ obtained in this way is in agreement with that obtained by imposing periodic boundary conditions.

For the Hubbard model, the real part of the optical conductivity obeys the following sum rule [27] (in units in which $\hbar = 1$),

$$\int_0^\infty Re\sigma_{\alpha\alpha}(\omega)d\omega = \frac{\pi e^2 \Delta^2}{2V} < 0|(-T_{\alpha})|0 >, \quad (3.4a)$$

in which $\Delta$ is the nearest-neighbor distance, which will be set to 1 in the numerical calculations, $V$ is the volume of the finite system, and $T_{\alpha}$ is the contribution of the hopping in the $\alpha$ direction to the total energy. We call it the kinetic energy of motion in the $\alpha$ direction. In a cubic system, the conductivity $\sigma$ is independent of the direction $\alpha$. If we take the convention
of setting $V = N\Delta^3$ where $N$ is the number of sites, Eq. (3.4a) can be simplified to

$$\int_0^\infty Re\sigma(\omega)d\omega = \frac{\pi e^2}{6N\Delta} < 0 | (-T) | 0 >,$$ (3.4b)

where $T$ is the total kinetic energy.

For a conventional metal, the real part of the conductivity satisfies the following $f$-sum rule [47]:

$$\int_0^\infty Re\sigma(\omega)d\omega = \frac{\pi ne^2}{2 m}$$ (3.5)

where $m$ is the free-electron mass. This relation can be obtained by integrating Eq. (3.2) over positive frequencies with the convention that the integral over positive frequencies includes $1/2$ of the $\delta$ function at $\omega = 0$; i.e., there is a contribution to (3.5) of $D/2$. The effective mass $m^*$ which appears in (3.3) is replaced by the free-electron mass $m$ in (3.5). Note that the right hand side of (3.5) is independent of the electron interaction while the right hand side of (3.4b) depends on the interaction. As a matter of fact, the right hand side of (3.4b) vanishes as $U \to \infty$. This discrepancy results from the one-band characteristics of the simple Hubbard model. The optical conductivity of an actual solid at energies of more than a few volts is dominated by the interband transitions which are not included in the one band Hubbard model. Even in many of the physical systems to which the Hubbard model is intend to apply (antiferromagnetic transition-metal compounds), the model cannot describe the charge-transfer transitions (oxygen $p$ states to metal $d$) which often define the onset of strong absorption [48]. We can
discuss the transitions across the Hubbard gap here, but it is not clear if there are experimental observations of this.

3.2 Theory and Calculational Methods

In this section we discuss the theory and methods of calculating the optical conductivity for a finite Hubbard system. Much of the discussion is based on Ref. [39].

We may obtain the current operator following Kohn’s method [26]. Consider a system perturbed by a position-independent vector potential \( \mathbf{A} \). Assume there is no external magnetic field in the system. The spin-magnetic field coupling term \( \mathbf{S} \cdot \mathbf{B} \) is neglected. Then the Hamiltonian of the whole system can be written as

\[
H = \sum_i \left[ \frac{1}{2m} (\mathbf{p}_i + \mathbf{A})^2 + V \right] + u
\]  

(3.6)

where \( m \) is the mass of the electrons, \( \mathbf{p}_i \) is the momentum operator for each electron, \( \mathbf{A} \) is the vector potential, \( V \) is the potential, and

\[
u = \frac{1}{2} \sum_{i \neq j} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|}
\]  

(3.7)

represents the electron-electron interaction term (see Eq. (1.3). A gauge transformation of the form \( \mathbf{A}' = \mathbf{A} + \nabla f(\mathbf{r}) \) with \( f(\mathbf{r}) = -\int_0^r \mathbf{A} \cdot d\mathbf{l} \) can be introduced to eliminate \( \mathbf{A} \) from Eq. (3.6) but modify the phase of the
orbitals \( \phi' = e^{-i\phi'(r)}\phi \). After the transformation we may obtain the Hubbard Hamiltonian with the perturbation \( A \) presents from Eq. (3.6),
\[
H = t \sum_{\langle ij \rangle, \sigma} e^{-i e A \cdot (R_i - R_j)} c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}. \tag{3.8}
\]

We see that the only difference between Eq. (3.8) and the ordinary Hubbard Hamiltonian (1.4) is that the hopping matrix elements in (3.8) are multiplied by a phase factor.

Assume the perturbation \( A \) is small. We expand the first term of (3.8) to the second order in \( A \). Then the current \( J_\alpha \) can be defined as
\[
J_\alpha = -\frac{\partial H}{\partial A_\alpha} = N(j_\alpha^{(P)} + j_\alpha^{(D)}). \tag{3.9}
\]

(\( \alpha \) is a rectangular component and \( N \) is the number of sites). The current consists of two parts: one is \( j_\alpha^{(P)} \) which is not dependent on \( A \) and is called the paramagnetic current; The other is \( j_\alpha^{(D)} \) which depends on \( A \) and is referred to as the diamagnetic current. We include only the nearest neighbor hopping so that \( R_i - R_j \) is a nearest-neighbor lattice vector, \( \Delta_{ij} \).

In the cubic system here, we set \( |\Delta| = 1 \), and \( \Delta_{ij} \) along a cube axis. For convenience, let \( A \) be in \( x \) direction. Then,
\[
j_x^{(P)} = \frac{i et}{N} \sum_{\langle ij \rangle, \sigma} \Delta_{ij, x} c_{i\sigma}^{\dagger} c_{j\sigma}, \tag{3.10a}
\]
\[
j_x^{(D)} = \frac{te^2}{N} A \sum_{\langle ij \rangle, \sigma} \Delta_{ij, x}^2 c_{i\sigma}^{\dagger} c_{j\sigma} = \frac{e^2 A}{N} T_x, \tag{3.10b}
\]
where $T_x$ is the kinetic energy due to the motion in the $x$ direction. Using the density matrix $\rho$, one then can find the real "observed" current

$$\langle j_x \rangle = \text{Tr}[\rho(p^{(P)}_{j_x} + p^{(D)}_{j_x})]. \tag{3.11}$$

One can evaluate the trace in (3.11) by a standard procedure [8,47] and retain only the first order terms in $A$ in order to obtain the complex conductivity tensor $\sigma_{\alpha\beta}$

$$\sigma_{\beta\alpha} = \frac{e^2}{iN(\omega + i\eta)} \langle T_{\alpha} \rangle_0 \delta_{\alpha\beta} + \frac{i}{\omega + i\eta} \Pi_{\alpha\beta}, \tag{3.12}$$

where $\eta$ is an infinitesimal positive quantity, $\langle \cdots \rangle_0$ indicates an average with the density matrix in the absence of the field (ground-state average at $T = 0$), and $\Pi_{\alpha\beta}$ is the current-current correlation function which is given by

$$\Pi_{\alpha\beta} = \frac{1}{N} \sum_m \langle 0 | j^{(P)}_{\beta} | m \rangle \langle m | j^{(P)}_{\alpha} | 0 \rangle \times \left[ \frac{1}{\omega + \omega_0 - E_m + i\eta} - \frac{1}{\omega + \omega_0 + E_m + i\eta} \right]. \tag{3.13}$$

In a cubic system, only the diagonal terms ($\alpha = \beta$) of $\sigma$ are not zero.

The complex conductivity may be separated into real part and imaginary part,

$$\sigma_{\alpha\alpha}(\omega) = \sigma_{R}(\omega) + i\sigma_{I}(\omega). \tag{3.14}$$
Let $\eta$ go to zero. We can find the real part and imaginary part of the conductivity as,

$$\sigma_R(\omega) = D\delta(\omega) + \frac{\pi}{3N\omega} \sum_m |<0| j|m>|^2 \delta(\omega + E_0 - E_m), \quad (3.15)$$

and

$$\sigma_I(\omega) = \frac{1}{3N\omega} \{ e^2 < -T > + \sum_m |<0| j|m>|^2 
\times \left( \frac{1}{\omega + E_0 - E_m} - \frac{1}{\omega - E_0 + E_m} \right) \}, \quad (3.16)$$

where the sum over $m$ becomes to a principle-value integral in the case of a bulk system. $\sigma_R$ is singular at $\omega = 0$. $D$ is the Drude weight which has the value

$$D = \frac{\pi}{N} \left[ e^2 < -T > + 2 \sum_m \frac{|<0| j_\alpha|m>|^2}{E_0 - E_m} \right]. \quad (3.17a)$$

The index $\alpha$ can be dropped for a cubic system, giving

$$D = \frac{\pi}{3N} \left[ e^2 < -T > + 2 \sum_m \frac{|<0| j|m>|^2}{E_0 - E_m} \right]. \quad (3.17b)$$

For a two-dimensional square lattice, the factor 3 in the denominator becomes 2.

In a finite system, we can avoid the singularities by retaining a small finite value for $\eta$. We use

$$\text{Re} \frac{1}{\omega \pm E_0 \mp E_m + i\eta} = \frac{\omega \pm E_0 \mp E_m}{(\omega \pm E_0 \mp E_m)^2 + \eta^2}.$$

The real dielectric function is obtained from $\sigma_I$ by (cgs units)

$$\epsilon_R(\omega) = 1 - 4\pi \sigma_I/\omega. \quad (3.18)$$
The real and imaginary parts of the conductivity are connected by the Kramers-Kronig relations. One of the relations is

$$\sigma_I(\omega) = -\frac{1}{\pi} P \int_{-\infty}^{\infty} \frac{\sigma_R(\nu)}{\nu - \omega} d\nu. \quad (3.19)$$

[and $\sigma_R(-\nu) = \sigma_R(\nu)$]. In the limit of $\omega \to \infty$, Eq. (3.19) gives the following result

$$\lim_{\omega \to \infty} [\omega \sigma_I(\omega)] = \frac{2}{\pi} \int_{0}^{\infty} \sigma_R(\nu) d\nu. \quad (3.20)$$

It then follows from (3.16) that

$$\int_{0}^{\infty} \sigma_R(\nu) d\nu = \frac{\pi}{6N} e^2 < -T >, \quad (3.4b)$$

which is the $f$-sum rule discussed in the Introduction.

When the ground state is non-degenerate, we can derive from (3.4b), (3.17b) and (3.16) that

$$\sum_{m} \frac{| < 0 | j | m > |^2}{E_m - E_0} = \frac{e^2}{2} < -T >. \quad (3.21)$$

This relation can also be obtained by using commutation rules, which holds under open boundary conditions, to evaluate the sum. However, Eq.(3.17b) then implies $D = 0$, as discussed previously.

Since our calculations are performed with open boundary conditions, the Drude weight $D$ calculated from Eq. (3.17b) must be zero. This is a useful check on the numerical calculations.
In our computer program, the Hamiltonian matrix is diagonalized to get the ground state energy and wavefunctions which are stored in memory and the real part of the conductivity is calculated according to Eq. (3.10a) and (3.15). \( \eta \) is set to a small positive number (0.05) to make the results finite. The Drude weight \( D \) is always zero in our case. We can use Eq. (3.17b) to check our calculated results.

3.3 Results

We calculated the optical conductivity in the half-filled band case, as well as for systems with one-hole and two-holes. In order to understand the results, we would like to return to Fig. 2 to look at the single particle eigenspectra first. There are four energy levels in Fig. 2, located at energies \(-3t, -t, t, \) and \(3t\), respectively. The highest level at \(3t\) and the lowest level at \(-3t\) are non-degenerate. The two at \(-t\) and \(t\) are triply degenerate. The symmetries of the levels from lowest to highest are \(\Gamma_1, \Gamma_5, \Gamma_{15}, \) and \(\Gamma_1\). If the sign of \(t\) is negative the order of the symmetries is reversed but nothing else changes. The current operator given in Eq. (3.10a) belongs to \(\Gamma_{15}\). When \(U = 0\), the lowest two levels are fully occupied in the half-filled case. This situation is reminiscent of a semiconductor rather than a metal. In the one- and two-hole cases, the second level is not completely filled: these cases correspond to metals.

As discussed in Sec. 3.2, the quantity \(< -T >\), the ground-state expectation value of the noninteracting part of the Hamiltonian is of great importance in the study of the optical conductivity. The total integrated weight
of the real part of the conductivity is directly proportional to \( < -T > /N \) (Eq. (3.4b)), where \( N \) is the number of sites. Table 2 gives the values of \( < -T > /N \) for different \( U \) and band fillings. The result show that as \( U \to \infty \), \( < -T > /N \) vanishes in the half-filled limit, indicating the disappearance of the optical absorption. However, this does not happen in other band fillings. When \( U = 0 \), \( < T > \) is simply the ground state energy of the system. It can be easily figured out by adding electrons to the single particle states listed in Fig. 2. The first two electrons go into the state with \( E = -3t \). The remainder enter the states with \( E = -t \). When \( U \) is nonzero but small, \( < -T > \) remains close to its value in the noninteracting limit, but as \( U \) increases (\( U > 6 \)), \( < -T > \) develop a maximum at \( n = 5 \).

Based on Eq. (3.4b) and (3.5), we would like to relate our data for \( < -T > \) to the quantity \( n/m^* \) [(electron density)/(effective mass)] near a metal-insulator transition. However, the small size of the system imposes two limitations on this consideration. First, a sharp transition is not to be expected even at \( T = 0 \) in a finite system, unless there is a symmetry change of the ground state due to a crossing of levels. This does not occur in the half-filled case in our model. Second, even a gradual transition may be partially obscured by the gaps in the single particle spectrum shown in Fig. 2.

In spite of these problems, our consideration may still lead us to some meaningful interpretations of our results. Since (for \( U \leq 4 \)), \( < -T > \) increases monotonically with an increasing number of particles for fixed \( U \), and also since the absorption for small \( U \) has a straightforward interpretation in
Table 2.

The ground-state expectation value of the negative of the first term in Eq. (1.4), $< -T > / N$ is given for all band fillings and selected values of $U$.

<table>
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<tr>
<th>$n$</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
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<td>0.75</td>
<td>0.875</td>
<td>1.0</td>
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</table>
terms of single-particle transitions, it is reasonable to define an effective mass as the ratio of \( < -T > \) for \( U = 0 \) and fixed \( n \) to that for nonzero \( U \):

\[
m^*(n, U) = \frac{< -T >_0}{< -T >_U}.
\]

(3.22)

The \( m^* \) here is not the usual effective mass of band theory because the band mass has been scaled out; rather, it is a quantity which measures the effect of interactions on the integrated optical absorption. Fig. 14 shows the results for \( m^* \) at different band fillings for \( U = 4 \). We see that for small \( U \), \( m^* \) is close to but always larger than unity for all \( n \).

For large \( U \), the situation is different. \( < -T > \) has a maximum at \( n = 5 \), and decreases rapidly as the half-filled limit is approached. The results for the spectral weight function described in Chapter 2 shows only a modest overall narrowing for the density of states at large \( U \). It is, therefore, reasonable for us to believe that the decrease of \( < -T > \) is due to the decrease of effective number of charge carriers. We believe that these data support the idea that a metal-insulator transition occurs only in the half-filled band case, and as \( n \to 0 \), rather than as \( m^* \to \infty \).

Next we look at the results for the optical conductivity. At \( U = 0 \), the only optical absorption occurs at \( \omega = 2 \) (for \( n = 6, 7, 8 \)), and corresponds to the transition between \( \Gamma'_{25} \) and \( \Gamma_{15} \) levels. As \( U \) increases, absorption is spread over a range of energies. In half-filled case, however, the absorption moves steadily to higher energies. Fig. 15 shows the calculated optical conductivity for \( U = 1, 4, 8, 12, \) and 100. The integrated weight of the absorption drops, as required by the data of Table 2. The factor of \( \omega^{-1} \) in Eq. (3.12) also plays a rule in this drop since the absorption moves to higher energies. When
Fig. 14. Variation of the effective mass defined by Eq. (3.22) with occupancy for $U = 4t$. The sharp change of slope at $n = 5$ is probably a finite-size effect.
Fig. 15a. Optical conductivity for the half-filled band case of $U = 1$. Curves are computed with a broadening ($\eta$) of 0.05. The Hubbard parameter $U$ and the frequency $\omega$ are given in units of the hopping integral $t$. 
Fig. 15b. Optical conductivity for the half-filled band case of $U = 4$. 
Fig. 15c. Optical conductivity for the half-filled band case of $U = 8$. 
Fig. 15d. Optical conductivity for the half-filled band case of $U = 12$. 
Fig. 15e. Optical conductivity for the half-filled band case of $U = 100$. 
$U > 8$ (roughly), antiferromagnetism is established in half-filled case in the sense that the antiferromagnetic structure factor is within $10\%$ of its limit as $U \rightarrow \infty$. The energy spectrum then has a separate, low-lying manifold of states corresponding to spin rearrangement. These states are not accessible from ground state by optical absorption. Transitions to a higher manifold whose states involve a real (as opposed to virtual) double occupancy are required for the absorption. These transitions need an energy of order of $U$. Therefore, if we plot the position of the lowest peak in the conductivity, as shown in Fig. 16, the curve will increase monotonically as $U$ increases. The real part of the dielectric function will show resonance behavior associated with the conductivity peaks.

We show our results in Fig. 17 for the one hole case. The conductivity is shown for $U = 1, 4, 8,$ and $12$. As observed previously, $D = 0$ as a consequence of open boundary conditions. At $U = 0$, the absorption is just a single peak located at $\omega = 2$, corresponding to the allowed single-particle transition. As $U$ increases, this peak broadens and splits. Fig. 16 plots the position of the lowest peak as a function of $U$. In addition, absorption develops at higher energies, and becomes associated with transitions into the upper Hubbard band.

Up to about $U = 6$ (note that the "bandwidth" is also 6), the lowest absorption peak remains close to $\omega = 2$. Evidently, this tells us that the optical absorption at the energy of single-particle transition persists until $U$ is about the size of the bandwidth. As $U$ increases further, this peak moves to lower energies. For $U \geq 10$, there is a clear separation of the lower and higher Hubbard bands. There are several absorption peaks in each band.
Fig. 16. Energy of the lowest (major) peak in the optical conductivity peak is shown as a function of $U$. Long-dashed line, half-filled band; solid line, one-hole case; short-dashed line, two-holes. All quantities are in units of $t$. 
Fig. 17a. Optical conductivity for one hole in the half-filled band for $U = 1$. 
Fig. 17b. Optical conductivity for one hole in the half-filled band for $U = 4$. 
Fig. 17c. Optical conductivity for one hole in the half-filled band for $U = 8$. 

Fig. 17d. Optical conductivity for one hole in the half-filled band for $U = 12$. 
We believe that this peak structure is a consequence of the finite size of the system. In the limit of bulk system, the absorption probably would be distributed more uniformly over both the lower and upper bands. From the comparison of the conductivity in the half-filled and one-hole cases at intermediate $U$ ($U = 8$, and 12), we see that doping leads to a transfer of absorption from higher to lower energy. The data of Table 2 shows that the integrated absorption is not constant with doping, but change is not large for $U \sim 6$ or 8, i.e., for values of $U$ similar to the bandwidth. The one-hole system remains metallic with a narrow quasiparticle band persisting to large $U$. In our case, the ground state becomes the Nagaoka ferromagnetic state [12] for $U > 39.5$. Since this is a noninteracting state, the absorption for $U > 39.5$ reverts to a single peak at $\omega = 2$, but now corresponding to a transition between $\Gamma_{15}$ and $\Gamma_1$ single-particle states.

Following Moreo and Dagotto [38], we define the scaled integrated absorption up to frequency $\omega$,

$$Z(\omega) = \frac{6N}{\pi e^2 < -T >} \int_0^\omega \sigma_R(\omega')d\omega'.$$

It follows from Eq. (3.4b) that $Z(\infty) = 1$. Fig. 18 shows the calculated results of $Z(\omega)$ for several values of $U$ in the one-hole case. When $U$ is small, almost all the absorption occurs in a small energy range near $\omega = 2$, as shown in Fig. 18(a) for $U = 2$. As $U$ increases, a plateau forms close to $Z = 1/2$ (Fig. 18(c) and 18(d)). This results from the separation of the lower and upper Hubbard bands. The plateau begin to build up at about $U = 8$. It shows up quite clearly when $U$ reaches 12. The Hubbard gap of the energy spectrum for spin-$\frac{1}{2}$ states at $n = 7$ forms at $U = 10$ (refer to Fig.4 in Ref.
**Fig. 18a.** Dimensionless integrated absorption $Z(\omega)$ [Eq. (3.23)] as a function of frequency for one hole in the half-filled band for $U = 2$. 
Fig. 18b. Dimensionless integrated absorption $Z(\omega)$ [Eq. (3.23)] as a function of frequency for one hole in the half-filled band for $U = 4$. 
Fig. 18c. Dimensionless integrated absorption $Z(\omega)$ [Eq. (3.23)] as a function of frequency for one hole in the half-filled band for $U = 8$. The dashed line indicates a plateau where the Hubbard gap develops.
Fig. 18d. Dimensionless integrated absorption $Z(\omega)$ [Eq. (3.23)] as a function of frequency for one hole in the half-filled band for $U = 12$. 
[20] or Fig. 8.5.4 in Ref. [47]). When this happens, the integrated absorption is about equally divided between upper and lower Hubbard bands.

As $U$ continues to increase, the plateau widens and the Hubbard gap approaches $U$. Then most of the integrated absorption is concentrated in the lower band.

Wagner, Hanke and Scalapino [39] have pointed out that the Drude weight can be estimated under open boundary conditions even if the $D$ calculated from Eq. (3.17a) is zero. This is done by integrating over the low-energy absorption ("Drude precursor") in the lower Hubbard band, which they interpret (see their Fig. 12) as the absorption in the lower Hubbard band. Their result, for a one dimension system, appears to agree well with the value of $D$ in the metallic case obtained when periodic boundary conditions are employed.

In our 3D system, some ambiguity may be encountered when we try to define the "Drude precursor" due to the complex multipeak structure of the conductivity. It is possible that some peaks at intermediate energies in the lower Hubbard band become a midinfrared feature in a large system [38,42], as seen in cuprate superconductors. We perform the integration mentioned above to get the Drude weight and find that the Drude weight has one-half of the total absorption when the Hubbard bands separate, and the full absorption for large $U$.

In the case of two-holes, the general picture is similar to that for one-hole. Fig. 19 shows the optical conductivity for four different values of $U$. The absorption begins at $U = 0$ with a single peak at $\omega = 2$, just as in the
Fig. 19a. Optical conductivity for two holes in a half-filled band for $U = 2$. 
Fig. 19b. Optical conductivity for two holes in a half-filled band for $U = 4$. 
Fig. 19c. Optical conductivity for two holes in a half-filled band for $U = 8$. 
Fig. 19d. Optical conductivity for two holes in a half-filled band for $U = 12$. 
one-hole case. This peak broadens and splits as $U$ increases. The lowest major absorption peak, whose position is shown in Fig. 16, move away from the energy of the single-particle transition more rapidly than in the one-hole case. For large $U$, beyond the range shown in Fig. 16, the position of the peak for two holes is at slightly higher energies than that for one-hole.

A Hubbard gap is apparent in the optical conductivity for two holes for somewhat smaller values of $U$ than for one hole. It can be seen at $U = 6$ for two holes, but is not seen for one hole until $U = 8$ or 10. This difference is probably a feature of the small system we consider in which the holes are spatially constrained. Probably a more significant result is that when $U$ is large enough so that the Hubbard bands are clearly separated, the widths of the lower bands are very nearly equal to 6, which is the single-particle bandwidth (compare Figs. 17(d) and 19(d)), in both cases. The manifold of two-particle states is wider than this, about 10. The states in the upper portion of this manifold are not accessible optically from the ground state. The results of the integrated absorption in two-hole case are shown in Fig. 20. These results are different from that in one-hole case. When the manifolds separate as $U$ increases, the integrated absorption associated with the lower manifold is about three times that associated with the upper manifold. Taking into account the data of Table 2 (and excluding the one hole case where $U = 100$ for which the ground state is the high spin state), this implies that the integrated absorption associated with the lower band is roughly twice as large in the two-hole case than for one hole. If the integrated absorption associated with the lower band is considered as an approximation to the Drude weight which is a quantity proportional to the
Fig. 20a. Integrated absorption $Z(\omega)$ [Eq. (3.23)] as a function of frequency for two holes in the half-filled band for $U = 2$. 
Fig. 20b. Integrated absorption $Z(\omega)$ [Eq. (3.23)] as a function of frequency for two holes in the half-filled band for $U = 4$. 
Fig. 20c. Integrated absorption $Z(\omega)$ [Eq. (3.23)] as a function of frequency for two holes in the half-filled band for $U = 8$. The dashed line indicates the plateau corresponding to the Hubbard gap.
Fig. 20d. Integrated absorption $Z(\omega)$ [Eq. (3.23)] as a function of frequency for two holes in the half-filled band for $U = 12$. 
number of carriers for large system, as seen in Eq. (3.3), we see that the
carriers should be considered as holes rather than electrons in our system.
This is in agreement with that of Ref. [42] for the 2D Hubbard model. We
believe that this result supports the view that the metal-insulator transition
is characterized by \( n \to 0 \) rather than \( n^* \to \infty \).

### 3.4 Conclusions

In this Chapter we investigated the frequency-dependent optical conduc­tivity of the simple Hubbard model in three dimensions by means of exact
numerical calculations for an eight-site cubic cluster. We obtain the results
of the conductivity for different interaction strengths \( (U) \) ranging from weak
coupling to strong coupling. The small size of the cluster made it necessary to
consider the specific features of this system, such as the actual single-particle
level spectrum, carefully in our analysis of the results.

Our results show that in the half-filled case, the optical absorption began
(for \( U = 0 \)) at \( \omega = 2 \), which corresponds to the energy of the lowest allowed
single-particle transition. As \( U \) increases, it moves to higher energies and
in the large \( U \) limit, it occurs near \( \omega = U \), resulting from transitions which
create a double occupancy.

In one-hole doping case, the absorption also starts with a single peak at
\( \omega = 2 \). As \( U \) increases, this peak splits into two portions whose intensity is
initially roughly equal, corresponding to transitions from the ground state
to lower and upper Hubbard bands, respectively. The splitting becomes
apparent around \( U \sim 10 \), i.e., somewhat larger than the overall width of
the single-particle states. As $U$ continues to increase, the Hubbard gap approaches $U$, the absorption is principally in the lower portion. However, in the specific geometry considered here, the ground state becomes to the Nagaoka high spin state when $U > 39.5$. The absorption reverts to a single peak at $\omega = 2$ again.

The results of absorption for two-hole doping case are qualitatively similar to those for one-hole, but have quantitative differences, especially in the magnitude of absorption. Beginning with a single peak at $\omega = 2$, the absorption splits into two portions at a somewhat smaller $U (U \sim 6)$ than for one-hole. The upper portion of the absorption is weaker by roughly a factor of 2 compared to the one-hole case.

In all cases, the integrated absorption is a monotonically increasing function of the number of electrons in the band when $U$ is small. Therefore, the interaction effects can reasonably be described in terms of an effective mass which increases with $U$. This pattern changes for large $U$, where the absorption decreases as the band-filling approaches the half-filled case. This is consistent with a picture in which the effective number of carriers goes to zero linearly with "doping", i.e., with the number of holes in the half-filled band.

Although details of the calculated optical conductivity depend on the specifics of the small cluster considered, many general features are the same regardless of those specifics. Comparison of our results for a small 3D system with the results for a $4 \times 4$ 2D system given by Ref. [42] shows some similar behavior which we believe is generic: For half filling, transitions occur only to states in the upper Hubbard band. When the system has holes, spectral
weight is transferred to lower energies. A Drude term appears and there is optical absorption within the lower Hubbard band, which may be related to the midinfrared feature observed in high-$T_c$ superconductors. Perhaps most importantly, the approximate linear dependence of the effective number of carriers on hole doping from the half-filled band for sufficiently large $U$ is also observed in the 2D case.
REFERENCES


[14]. See, for example, Ref. 9.


[17]. D. P. Chen, Ph.D dissertation.


APPENDIX

COMPUTER PROGRAMS

A.1 Spectral Weight Function .................................................... 96
A.2 Conductivity ................................................................. 128
A.1 Spectral Weight Function

```
1 //PHTANL1  JOB (1103,69869,100,22), 'PHTANL', MSGLEVEL=(1,1),
2 //   MSGCLASS=S, CLASS=H
3 /*JOBPARM SHIFT=D
4 //*/AFTER GRD12
5 //*/ROUTE PRINT RMT4
6 //S1 EXEC VSF2CLG, REGION.FORT=SM,
7 //   PARM.FORT='SOURCE, NOTERM, OPT(3), VEC',
8 //   PARM.LKED='NOMAP, NOXREF, LIST, LET, AMODE=ANY',
9 //   PARM.GO='NOXUFLOW',
10 //   REGION.GO=999M, TIME.GO=999,
11 //   LIB='SYS1.ESVVLIB'
12 //FORT.SYSIN DD *
13 @PROCESS DC(C,Y,C1)
14 C-------------------------------------------------------------------
15 C FOLLOWING PROGRAM TO PERFORM HUBBARD MODEL CALCULATION FOR
16 C CUBIC CLUSTER BY MEANS OF SYMMETRIZED BASIS TO GET THE
17 C SPECTRAL WEIGHT FUNCTION FOR A HALF-FILLED CLUSTER.
18 C NSITE=# OF SITES; NTL=# OF TOTAL ELECTRONS
19 C NPRTL=TOTAL NUMBER OF NEAREST NEIGHBOR PAIRS
20 C UIN IS PARAMETER IN HUBBARD MODEL; THOP IS T
21 C EIGENENERGIES ARE STORED IN EN ARRAY
22 C ELIM7 & ELIM9: UPPER LIMIT OF ENERGY SPECTRA FOR 7 & 9
23 C ELECTRON SYSTEMS, RESPECTIVELY;
24 C EMINT: GROUND STATE ENERGY OF THE 8 ELECTRON SYSTEM;
25 C D: WIDTH PARAMETER;
26 C RESULTS ARE STORED IN FILES GKV1, GKV2, GKV3 AND GKV4,
27 C CORRESPONDS TO FOUR WAVE VECTORS.
28 C-------------------------------------------------------------------
29 C IMPLICIT REAL*8(A-H, O-Z)
30 COMPLEX*16 GRE1(4,300,10), DENW, GR1(4,300), GR2(4,300),
31 *GRE2(4,300,10)
32 DIMENSION WK(1300), ZDUM1(650,5000), ZDUM2(650,5000)
33 DIMENSION ZDUM3(650,5000)
34 DIMENSION ENS(3,101), EN1(650), EN2(650), EN3(650)
35 DIMENSION WEIT(8,650,8), NWEIT(8,650,8), MDIM(8), ZFO(10)
36 DIMENSION HWV(211575), ENW(650), ZDUMW(650,650)
37 DIMENSION NPR(50,2), NDIF1(8), NDIF2(8)
38 DIMENSION NSUP1(100,8), NSDN1(100,8), NSUP2(100,8), NSDN2(100,8)
```
DIMENSION NSUP3(100,8),NSDN3(100,8),NSUP(100,8),NSDN(100,8)
DIMENSION AW1(4,300,10),AW2(4,300,10),NSU(58),NSD(58)
DIMENSION NUIMIN(IO),ND1MIN(10),NME(10),EL(10),EL1(10)
DIMENSION NSUPBS(IOO),NSDNBS(100),NPRS(10,2)
DIMENSION CDN1(4,650,650),CIDN(4,650,650)
DIMENSION NSM1(3),NSM2(300),NSM3(300)
COMMON /C/ZDUM1, ZDUM2,CIDN
COMMON /C1/CDN1,ZDUM3,GRE1,GRE2
COMMON /C2/NPR, NSITE, NPRTL
COMMON /C3/NSUP1,NSDN1,NSUP2,NSDN2
COMMON /Y/HWV,ZDUMU, ENW
CALL ERRSET(208,0,-1,0,1,1)
C==========================================================
C DEFINE SYSTEM
NDIMX=650
NDIMX2=2*NDIMX
NSITE=8
C ------------------ THIS PARAMETER MUST AGREE WITH # OF SITES ------
C PARAMETER NDIMX MUST AGREE WITH DIMENSION OF HW
C ---------- CHECK THE PARAMETERS ABOVE ------------------
READ(5,100)NPRTL
WRITE(6,100)
DO 1  1=1,NPRTL
READ(5,102)NPR(I,1),NPR(I,2)
1 CONTINUE
102 FORMAT(2I5)
READ(5,101)U
READ(5,106)NTH0P,THOPIN,DTHOP
READ(5,102)NTLIN, NTLFL
106 FORMAT(I5,2F10.6)
READ(5,*0EMINT
NC0RMX=30
LSTMX=100
DO 9999 NTL=NTLIN,NTLFL
THOP=THOPIN
IF(NTL-NSITE)1000,1000,1001
1000 NUST=NTL+1
NMMAX=NTL
GO TO 1002
1001 NUST=NSITE+1
NMMAX=2*NSITE-NTL
1002 DO 310 IU=1,NTHOP
WRITE(6,6788) NTL
WRITE(16,6788) NTL
WRITE(6,6789)U,THOP
WRITE(16,6789)U,THOP
6791 FORMAT(IX,' THE ENERGY UNIT IS T IN HUBBARD MODEL')
6788 FORMAT(IX,' THE FOLLOWING RESULTS ARE ABOUT CUBIC CLUSTER WITH
* ',I4,' ELECTRONS ')
6789 FORMAT(IX,' HUBBARD MODEL CALCULATION WHEN U=',F10.4,5X,'T=',
* F10.4,5X)
10483 FORMAT(IX, F6.2,4X,F6.2)
100 10483 FORMAT(IX, F6.2,4X,F6.2)
----START CALCULATION IN DIFFERENT Z COMPONENT OF SPIN SUBSPACES ----
IRC=0
DO 300 IRAN=1,NTL
NUP=NUPST-IRAN
IF(NUP.LE.0)GO TO 300
NDN=NTL-NUP
IF(NDN.GT.NUP)GO TO 300
IRANMX=IRAN
JQ1=1
JQ2=0
JQ3=0
DO 2001 IQXY=1,NDIM
EN1(IQXY)=0.0D0
EN2(IQXY)=0.0D0
EN3(IQXY)=0.0D0
2001 EN1(I)=110.0D0
---- PERFORM CALCULATION FOR N-1, N, AND N+1 ELECTRON SYSTEMS ------
DO 3070 NAD=1,3
IF(NAD.EQ.1) THEN
NUP1=NUP
NDN1=NDN
ELSEIF(NAD.EQ.2) THEN
NDN=NDN+1

NUP2 = NUP
NDN2 = NDN
ELSEIF (NAD.EQ.3) THEN
NDN = NDN - 2
NUP3 = NUP
NDN3 = NDN
ENDIF
IF (NDN .GT. NSITE) GOTO 3070
IF (NDN .LT. 0) GOTO 3070
100 FORMAT (I5)
101 FORMAT (F10.5)

C ------------------------ GENERATE BASIS FUNCTIONS ------------------------
CALL GENLST (NUP, NSITE, JUP, NSUP)
CALL GENLST (NDN, NSITE, JDN, NSDN)

C -------------------------------
NDIM = JUP * JDN
ELSEIF (NAD.EQ.1) THEN
NDIM11 = NDIM
JUP1 = JUP
JDN1 = JDN
DO 360 N = 1, NSITE
DO 361 I = 1, JUP1
361 NSUP1 (I, N) = NSUP (I, N)
DO 362 I = 1, JDN1
362 NSDN1 (I, N) = NSDN (I, N)
360 CONTINUE
ELSEIF (NAD.EQ.2) THEN
NDIM22 = NDIM
JUP2 = JUP
JDN2 = JDN
DO 370 N = 1, NSITE
DO 371 I = 1, JUP2
371 NSUP2 (I, N) = NSUP (I, N)
DO 372 I = 1, JDN2
372 NSDN2 (I, N) = NSDN (I, N)
370 CONTINUE
ELSEIF (NAD.EQ.3) THEN
NDIM33 = NDIM
JUP3 = JUP
JDN3 = JDN
DO 380 N = 1, NSITE
DO 381 I = 1, JUP3
NSUP3(I,N) = NSUP(I,N)
DO 382 I = 1, JDN
NSDN3(I,N) = NSDN(I,N)
CONTINUE
ENDIF
C IF(NAD.EQ.3) WRITE(16,103) NUP, JUP, NDN, JDN, NDIM, NSITE
WRITE(6,103) NUP, JUP, NDN, JDN, NDIM, NSITE
103 FORMAT(1X, 'NUP, JUP, NDN, JDN, NDIM, NSITE=', I5)
C FIND THE ATOMIC SPINS ON EACH SITE
C IF(THOP NE 0.01) GOTO 200
C JQ = 0
DO 200 IA = 1, JUP
DO 200 IB = 1, JDN
C !!! IT'S HERE !!!
WRITE(6,104) JQ, (NSUP(IA,K), K = 1, NSITE), (NSDN(IB,K), K = 1, NSITE)
104 FORMAT(I8, 3X, 8I3, 3X, 8I3)
C ---------- CONVERT BASIS FUNCTIONS TO BINARY CODE -------------
CALL TRANS(JUP, NSITE, NSUP, NSUPBS)
CALL TRANS(JDN, NSITE, NSDN, NSDNBS)
C ---------- FORM SYMMETRIZED BASIS FUNCTIONS -------------------
CALL SYBASE(WEIT, NWEIT, MDIM, NDIM, NSUP, NSDN, NSUPBS
1, NSDNBS, JUP, JDN, NSITE)
C -------------------------------------------------------------
778 FORMAT(IX, 'TEST=', 28F8.4)
2021 FORMAT(1X, 'THE DIM OF SYMMETRIZED STATES ARE', 2I9)
DO 7777 IXYP = 1, 8
NDIM1 = NDIM(IXYP)
WRITE(6,2021) IXYP, NDIM1
NDM2 = NDIM1*(NDIM1+1)/2
IF(NDIM1.EQ.0) GOTO 7777
DO 9100 I = 1, NDIM1
ENW(I) = 0.000
DO 9100 J = 1, NDIM1
9100 ZDUMW(I,J) = 0.000
DO 9113 IAB = 0
9113 HWV(I) = 0.000
IAB = IAB + 1
C ---------------- GENERATE HAMILTONIAN -------------------------
DO 9230 IA = 1, NDIM1
DO 9230 JB = IA, NDIM1
9230 IA = IA + 1
DO 9220 I=1,8
I1=NWEIT(IXYP,IA,I)
IF(I1.EQ.0) GOTO9220
DO 9221 J=1,8
J1=NWEIT(IXYP,JB,J)
IF(J1.EQ.0) GOTO9221
X=HIAB(I1,J1,JDN,U,THOP,NSUP,NSDN,NUP,NDN)
HWV(IAB)=HWV(IAB)+WEIT(IXYP,IA,I)*WEIT(IXYP,JB,J)*X
9221 CONTINUE
9220 CONTINUE
9230 CONTINUE
C=========================================================================
3859 FORMAT(1X,' THE HAMILTONIAN IS FOLLOWS')
C --------------DIAGONALIZATION BEGIN -------------------------------
C CALL EIGRS(HWV, NDIM1,2,ENW, ZDUMW,NDIMX,WK,IER)
CALL DSLEV(1,HWV, ENW,ZDUMW, NDIMX,NDIM1,WK,NDIMX2)
C ---------------STORE EIGENVALUES AND WAVEFUNCTIONS----------------------
DO 7830 I=1,NDIM1
IF(NAD.EQ.1) THEN
IF(ENW(I)-EN1(JQ1).GT.1.0D-8)GOTO 838
IF(ABS(ENW(I)-EN1(JQ1)).LT.1.0D-8) JQ1=JQ1+1
IF(ABS(ENW(I)-EN1(JQ1)).GT.1.0D-8.AND.JQ1.GT.1) JQ1=1
DO 9101 J=1,NDIM
9101 ZDUM1(JQ1,J)=0.0D0
EN1(JQ1)=ENW(I)
NSM1(JQ1)=IXYP
DO 7820 J=1,NDIM1
MN=NWEIT(IXYP,J,K)
IF(MN.EQ.0) GOTO7820
ZDUM1(JQ1,MN)=ZDUM1(JQ1,MN)+WEIT(IXYP,J,K)*ZDUMW(J,I)
7820 CONTINUE
838 CONTINUE
ELSEIF(NAD.EQ.2.AND.ENW(I).LE.ELIM9) THEN
JQ2=JQ2+1
DO 9102 J=1,NDIM
9102 ZDUM2(JQ2,J)=0.0D0
EN2(JQ2)=ENW(I)
NSM2(JQ2)=IXYP
DO 7821 J=1,NDIM1
MN=NWEIT(IXYP,J,K)
7821 CONTINUE
838 CONTINUE
IF(MN.EQ.0) GOTO7821
ZDUM2(jq2,MN)=ZDUM2(jq2,MN)+WEIT(IXYP,J,K)*ZDUMW(J,I)
CONTINUE
ELSEIF(NAD.EQ.3.AND.ENW(I).LE.ELIM7) THEN
JQ3=JQ3+1
DO 9103 J=1,NDIM
ZDUM3(JQ3,J)=0.0D0
EN3(JQ3)=ENW(I)
NSM3(JQ3)=IXYP
DO 7822 J=1,NDIM1
DO 7822 K=1,8
MN=NWEIT(IXYP,J,K)
IF(HN.EQ.0) GOTO7822
ZDUM3(JQ3,MN)=ZDUM3(JQ3,MN)+WEIT(IXYP,J,K)*ZDUMW(J,I)
CONTINUE
ELSE
GOTO 7830
ENDIF
7830 CONTINUE
7777 CONTINUE
C WRITE(6,*)'jqi',jqi
C-------------- OUTPUT EIGENENERGIES ----------------------
WRITE(6,6601)
WRITE(6,*)' ENl',(EN1(I),I=1,jqi)
IF(NAD.NE.3) GOTO 3070
WRITE(16,6601)
DO 7790 I=1,NDIM,5
14=1+4
IF(14.GT.NDIM) I4=NDIM
WRITE(6,105)1,(EN(KI),KI=I,14)
WRITE(16,105)1,(EN1(KI),KI=I,14)
7790 CONTINUE
WRITE(6,*) ' ENl',(ENl(I),I=1,jqi)
105 FORMAT(I5,15E20.8)
6601 FORMAT(IX,' THE EIGENENERGIES ARE')
C WRITE(6,86)(NSUP1(1,I),I=1,NSITE)
C WRITE(6,86)(NSDN1(1,I),I=1,NSITE)
NM=0
DO 653 I3=1,JUP3
DO 653 J3=1,JDN3
NM=NM+1
WRITE(6,86)(NSUP3(NM,I),I=1,NSITE)
WRITE(6,86)(NSDN3(NM,I),I=1,NSITE)
WRITE(6,86)JUP1,JDN1,JUP2,JDN2,NUP2,NDIM11,NDIM22
DO 253 I=1,8
WRITE(6,*)' ZDUM2',(ZDUM2(8,JJ),JJ=1,NDIM22)
WRITE(6,*)' ZDUM1',(ZDUM1(8, JJ),JJ=1,NDIM11)
WRITE(6,*)' ZDUM3',(ZDUM3(8, JJ),JJ=1,NDIM33)

----------CALCULATE MATRIX ELEMENTS--------------------------------
CALL SPEFC(JUP1,JDN1,JUP2,JDN2, NSITE, NUP2, NDIM11,NDIM22,JQI,JQ2,
INK,NSUP1,NSDN1,NSUP2,NSDN2)
IF(IRAN.EQ.(NTL/2+1)) THEN
WRITE(6,*'THE SYM. AND ENG OF THE GRD STATE',(NSM1(ISM), EN1(ISM),
*ISM=1,JQ1)
WRITE(6,*'K QJ2 NSYM EN2 DW1 CIDN'
DO 244 I=1,Q2
IF(DABS(EN2(I)-EMINT-U).GT.4.DO) GOTO 244
DW1=EN2(I)-EMINT
WRITE(6,443)1,NSM2(I),EN2(I),DW1,(CIDN(K,JQI,1),K=1,NK)
244 CONTINUE
ENDIF
ICMAX=MAX(JQ1, JQ3)
JCMAX=MAX(NDIM11,NDIM33)
DO 517 IC2=1,JCMAX
DO 517 IC1=1,ICMAX
ZDUM2(IC1,IC2)=ZDUM1(IC1,IC2)
517 ZDUM1(IC1,IC2)=ZDUM3(IC1,IC2)
DO 518 IQ2=1,JQ2
DO 518 IQ1=1,Q1
DO 518 IK=1,NK
CDN1(IK,IQ1,IQ2)=CIDN(IK,IQ1,IQ2)
518 CIDN(IK,IQ1,IQ2)=0.DO
CALL SPEFC(JUP3,JDN3,JUP1,JDN1,NSITE,NSUP2,NSUP3,NSDN1)
INK,NSUP3,NSDN3,NSUP1,NSDN1)
IF(IRAN.EQ.(NTL/2+1)) THEN
WRITE(6,*'K QJ3 NSYM EN3 DW CIDN'
DO 243 I=1,Q3
IF(DABS(EN3(I)-EMINT).GT.4.DO) GOTO 243
DW1=EN3(I)-EMINT
WRITE(6,443)1,NSM3(I),EN3(I),DW1,(CIDN(K,I,JQ1),K=1,NK)
CONTINUE
ENDIF
FORMAT(1X,20I5)
FORMAT(1X,2I5,2F10.5,4E16.5)
----------------------------------------------------------
WRITE(6,*)' ENl ',(ENl(I),I=1,JQ1)
DO 675 IK=1,NK
DO 675 IQ1=1,JQ1
WRITE(6,*),'CIDN',IK,(CIDN(IK,IQ3,IQ1),IQ3=1,JQ3)
DO 775 IK=1,NK
DO 775 IQ2=1,JQ2
WRITE(6,*),'CDN1',IK,(CDN1(IK,IQ1,IQ2),IQ1=1,JQ1)
FIND THE MIN ENERGY IN THE SUBSPACE -----------------------
EMIN1=EN1(1)
NMIN=1
NME(1)=1
IF (JQ1.EQ.1) GOTO 3701
DO 3700 IXY=2,JQ1
WRITE(6,*),EN1(IXY),EN2(IXY)
IF (DABS(EMIN1-EN1(IXY)).LT.1.0D-12) GOTO 3721
IF (EMIN1.LT.EN1(IXY)) GOTO 3700
EMIN1=EN1(IXY)
NMIN=NMIN+1
NME(NMIN)=IXY
GOTO 3700
3721 NMIN=NMIN+1
NME(NMIN)=IXY
CONTINUE
3701 NMIN=1
NME(1)=IXY
GOTO 3700
372 EMIN2=EN2(1)
EMIN3=EN3(1)
DO 4000 J2=2,JQ2
IF(DABS(EN2(J2)-EMIN2).LT.1.0D-12) GOTO 4000
IF(EN2(J2).LT.EMIN2) EMIN2=EN2(J2)

DO 5000 J3=2,JQ3
IF(DABS(EN3(J3)-EMIN3).LT.1.0D-12) GOTO 5000
IF(EN3(J3).LT.EMIN3) EMIN3=EN3(J3)

ELI(IRAN)=EMIN2
WRITE(6,*),'EG', EMIN1, EHIN2, EMIN3
C END OF EMIN ; BEGINNING OF GENERATING SPECTRAL WEIGHT FUNCTION

DO 404 K=1,NK
DO 404 IG=1,NW
GRE1(K,IG,IRAN)=(0.DO,0.DO)
GRE2(K,IG,IRAN)=(0.DO,0.DO)
AW1(K,IG,IRAN)=0.DO
AW2(K,IG,IRAN)=0.DO
WRITE(6,*),'# OF EIGENSTATES',jqi,jq2,JQ3
DO 20 1=1,jq2
WRITE(6,*)CIDN(1,1)
DO 254 IK=1,NK
DO 254 jq=l,jq2
WRITE(6,*)IK,jq,(CDN1(IK,iq,jq),iq=l,jqi)
WRITE(6,*)jqi,jq2,jq3
UM=U/2.DO
DSFM=O.DO
DO 414 K=1,NK
DO 414 IG=1,NW
GR1(K,IG)=(0.DO,0.DO)
GR2(K,IG)=(0.DO,0.DO)
CONTINUE

IF(jqi.EQ.0) GOTO 98
DO 401 IS=l,jqi
EBEJ=1.DO
DSFM=DSFM+EBEJ
IF(jq2.EQ.0) GOTO 99
DO 403 JS=l,jq2
W=WIN
DE=EN1(IS)-EN2(JS)
WRITE(6,*),'DE',EN1(IS),EN2(JS),DE
DO 402 IG=1,NW
DO 405 K=1,NK
RDEN=W+EN1(IS)-EN2(JS)+UM
DENW=DCMPLX(RDEN,D)
\begin{verbatim}
GR1(K,IG)=GR1(K,IG)+EBEJ*DBS(DN1(K,IS,JS))*2/DENW
CONTINUE
W=W+DW
CONTINUE
IF(JQ3.EQ.0) GOTO 401
DE=EN1(IS)-EN2(JS)
WRITE(6,*)EN1(IS),EN2(JS),DE
DO 406 KS=1,JQ3
    W=WIN
    DO 407 IG=1,NW
        DO 408 K=1,NK
            RDEN=W+EN3(KS)-EN1(IS)+UM
            DENW=DCMPLX(RDEN, D)
            GR2(K,IG)=GR2(K,IG)+EBEJ*DBS(DN(K,KS,IS))*2/DENW
        408 CONTINUE
    407 W=W+DW
  406 CONTINUE
  401 CONTINUE
  408 CONTINUE
  407 W=W+DW
  406 CONTINUE
  401 CONTINUE
DO 409 K=1,NK
    DO 409 IG=1,NW
        GR1(K,IG)=GR1(K,IG)+GR1(K,IG)
        DO 586 I1=1,IG
            WRITE(6,*)GR1(1,IG),GR2(1,IG)
    586 PI=3.1415926
    IF(NUP1.EQ.NDN1) GOTO 97
    ZFO(IRAN)=ZFO(IRAN)+2.0*DSFM
    DO 417 K=1,NK
        DO 416 IG=1,NW
            GRE1(K,IG,IRAN)=GRE1(K,IG,IRAN)+2.0*GR1(K,IG)
            AW1(K,IG,IRAN)=-DIMAG(GRE1(K,IG,IRAN))/PI
            AW2(K,IG,IRAN)=DIMAG(GRE2(K,IG,IRAN))/PI
            WRITE(6,*)'AW',K,IG,AW(K,IG,IRAN),ZFO(IRAN)
        416 CONTINUE
    417 CONTINUE
GOTO 98
  97 ZFO(IRAN)=ZFO(IRAN)+DSFM
  98 CONTINUE
\end{verbatim}
AW2(K,IG,IRAN)=-DIMAG(GRE2(K,IG,IRAN))/PI
C WRITE(6,*,'(A,W(K,IG,IRAN),ZFO(IRAN))
516 CONTINUE
515 CONTINUE
98 CONTINUE
IRC=IRC+1
307 CONTINUE
300 CONTINUE
98 CONTINUE
3134 FORMAT(IX,'THE TOTAL POSSIBLE CONFIGURATION OF NUP&NDN IS',I4,3X,'
*IIRANMX=',I4)
301 NMIN=1
EMIN=EL(1)
WRITE(6,3134) IRC,IRANMX
DO 299 IRAN=1,IRANMX
IF(ELCIRAN).GE.EMIN)GO TO 299
EMIN=EL(IRAN)
NMIN=IRAN
299 CONTINUE
DO 3710 IY=1,IRC
3710 WRITE(6,3711) EL(IY),NU1MIN(IY),ND1MIN(IY)
3711 FORMAT(IX,'THE POSSIBLE MIN ENERGY IS ',E20.5,'WHEN NUP=',I4,3X,'N
*DN=',I4)
WRITE(6,111) EMIN,NU1MIN(NMIN),ND1MIN(NMIN)
111 FORMAT(IX,'THE MIM ENERGY IS',E20.5,'WHEN NUP=',I4,3X,'NDN=',I4)
WRITE(6,112)
112 FORMAT(IX,'IU,U,THOP,T,<E>,SPH,MAGX,MAGXEXT,ZFO FOLLOW')
C FORMAT(IX,'IU,U,THOP,T,<E>,SPH,MAGX,MAGXEXT,ZFO FOLLOW')
C ============= IT'S HERE ===============
WRITE(6,3534)
3534 FORMAT(2X,'THE T AND SPIN-CO-FUNCTION OF Z-COMPONENT ')
DO 412 IK=1,NK

C ------------------------OUTPUT RESULTS ---------------------
NTL=NTL-1
DO 2121 IG=1,NW
DO 2121 K=1,NK
AW1(K,IG,NMIN)=AW1(K,IG,NMIN)/ZFO(NMIN)
GRE1(K,IG,NMIN)=GRE1(K,IG,NMIN)/ZFO(NMIN)
AW2(K,IG,NMIN)=AW2(K,IG,NMIN)/ZFO(NMIN)
2121 GRE2(K,IG,NMIN)=GRE2(K,IG,NMIN)/ZFO(NMIN)
WRITE(6,117) NTL,U,THOP,ELIM9,ELIM7
DO 412 IK=1,NK
NC=20+IK
WRITE(6,*) 'THE WAVE VECTOR K', IK
WRITE(NC,117) NTL, U, THOP, ELIM9, ELIM7
WRITE(NC,118) IK, T, D
W=WIN
DO 410 IG=1,NW
   AW=AW1(IK,IG,NMIN)+AW2(IK,IG,NMIN)
WRITE(NC,119) IG, W, AW1(IK,IG,NMIN), AW2(IK,IG,NMIN), AW
WRITE(6,119) IG, W, AW1(IK,IG,NMIN), AW2(IK,IG,NMIN), AW
410 W=W+DW
412 CONTINUE
WRITE(NC,115)
WRITE(6,115)
119 FORMAT(IS,F10.5,9E16.5)
118 FORMAT(IS, ' ', I3, 'X ', 'T=', I3, 'X ', 'D=', F8.4)
C WRITE(2,115)
C WRITE(3,115)
WRITE(6,115)
WRITE(23,115)
WRITE(24,115)
115 FORMAT(IS, ' END OF DATA. ')
STOP
END
C---------------------------------------------------------------------
QPROCESS DC(C,D)
0=====================================================================
C THIS FUNCTION GIVE THE <IA|H|IB> FOR PARAMETER U,T IN THE H
FUNCTION HIAB(IA,IB,JDN,U,T,NSUP,NSDN,NUP,NDN)
IMPLICIT REAL*8(A-H,O-Z)
DIMENSION NSUP(100,8),NSDN(100,8),NPR(50,2),NDIF1(8),NDIF2(8)
COMMON /C1/NSUP,NSDN
COMMON /C2/NPR,NSITE,NPRTL
333 HIAB=0.000
CALL FUD(IA,IAU,IAD,JDN)
CALL FUD(IB,IBU,IBD,JDN)
IF(IA.NE.IB) GOTO 20
IF(NDN.EQ.0) GO TO 999
DO 10 I=1,NSITE
109

544  IF(NSUP(IAU,I).EQ.1.AND.NSDN(IAD,I).EQ.1)HIAB=HIAB+U
545  10 CONTINUE
546  GOTO 999
547  20 ISUM1=0
548     ISUM2=0
549     ISUM3=0
550     ISUM4=0
551  DO 30 I=1,NSITE
552     NDIF1(I)=NSUP(IAU,I)-NSUP(IBU,I)
553     NDIF2(I)=NSDN(IAD,I)-NSDN(IBD,I)
554     ISUM1=ISUM1+NDIF1(I)
555     ISUM2=ISUM2+NDIF2(I)
556     ISUM3=ISUM3+IABS(NDIF1(I))
557     ISUM4=ISUM4+IABS(NDIF2(I))
558  30 CONTINUE
559  IF(ISUM3.GT.2) GO TO 999
560  IF(ISUM4.GT.2) GO TO 999
561  IF(ISUM1.NE.0) GO TO 999
562  IF(ISUM2.NE.0) GO TO 999
563  IF(ISUM3.EQ.2.AND.ISUM4.EQ.2)GO TO 999
564  C ONE MOVE HAS OCCURRED. IS IT A NEAREST NEIGHBOR PAIR?
565  IF(ISUM3.EQ.0) GO TO 100
566     MUS1=0
567     MUS2=0
568     MX=0
569  DO 40 ME=1,NSITE
570     MX=MX+1
571  IF(MUS1.NE.0)GO TO 45
572  IF(NDIF1(ME).NE.0)MUS1=MX
573  GO TO 40
574  45 IF(NDIF1(ME).NE.0)GO TO 41
575  40 CONTINUE
576  GO TO 999
577  41 MUS2=MX
578     IPRU=0
579  DO 50 MF=1,NRTL
580     IX=NPR(MF,1)-MUS1
581     IY=NPR(MF,2)-MUS2
582  IF(IY.NE.0)GO TO 55
583  IF(IY.NE.0)GO TO 55
584     IPRU=1
585  GO TO 51
586 55 IX=NPR(MF,1)-MUS2
587  IY=NPR(MF,2)-MUS1
588  IF(IX.NE.0)GO TO 50
589  IF(IY.NE.0)GO TO 50
590  IPRU=1
591  GO TO 51
592  50 CONTINUE
593  IF(IPRU.NE.1)GO TO 999
594  51 CALL SIGN(SGN,NUP,NSUP,MUS1,MUS2,IAU)
595  GO TO 998
596  100 MDS1=0
597  IF(NDN.EQ.0)GO TO 999
598  MX=0
599  MDS2=0
600  DO 145 ME=1,NSITE
601  MX=MX+1
602  IF(MDS1.NE.0)GO TO 140
603  IF(NDIF2(ME).NE.0)MDS1=MX
604  GO TO 145
605  140 IF(NDIF2(ME).NE.0)GO TO 146
606  145 CONTINUE
607  GO TO 999
608  146 MDS2=MX
609  IPRD=0
610  DO 155 MF=1,NPRTL
611  IX=NPR(MF,1)-MDS1
612  IY=NPR(MF,2)-MDS2
613  IF(IX.NE.0)GO TO 150
614  IF(IY.NE.0)GO TO 150
615  IPRD=1
616  GO TO 151
617  150 IX=NPR(MF,1)-MDS2
618  IY=NPR(MF,2)-MDS1
619  IF(IX.NE.0)GO TO 155
620  IF(IY.NE.0)GO TO 155
621  IPRD=1
622  GO TO 151
623  155 CONTINUE
624  IF(IPRD.NE.1)GO TO 999
625  151 CALL SIGN(SGN,NDN,NSDN,MDS1,MDS2,IAD)
626  998 HIAB=T*SGN
627  999 RETURN
SUBROUTINE SYBASE(WEIT, NWEIT, MDIM, NDIM, NSUP, NSDN, NSUPBS, JUP, JDN, NSITE)

IMPLICIT REAL*8(A-H,O-Z)

DIMENSION WEIT(8,650,8), NWEIT(8,650,8), CX(8,8)

DIMENSION NWEIT1(650,8), NSUPBS(100), NSDNBS(100)

DIMENSION WEIT1(650,8)

DIMENSION NSUP(100,8), NSDN(100,8), MDIM(8)

DIMENSION NSUSED(100), NUP(8), NDN(8), NUP1(8), NDN1(8)

DIMENSION WS(8), NS(8), WFS(8), NFS(8), NSUM(8), NSUM1(8), WSUM(8)

DIMENSION MUPF(8), MDNF(8), WCS(8)

DATA CX/1.000, 1.000, 1.000, 1.000, 1.000, 1.000, 1.000, 1.000,
* 1.000, 1.000, 1.000, 1.000, -1.000, -1.000, -1.000, -1.000,
* 1.000, 1.000, -1.000, -1.000, 1.000, 1.000, -1.000, -1.000,
* 1.000, -1.000, 1.000, 1.000, -1.000, -1.000, -1.000, -1.000,
* 1.000, 1.000, -1.000, -1.000, -1.000, 1.000, 1.000, -1.000,
* 1.000, -1.000, -1.000, 1.000, 1.000, -1.000, -1.000, -1.000,
* 1.000, -1.000, -1.000, -1.000, -1.000, -1.000, 1.000, 1.000,
* 1.000, -1.000, -1.000, -1.000, 1.000, -1.000, -1.000, -1.000/.

WRITE(6,'(I8)') JUP, JDN, NSITE

DO 933 I=1,8

DO 933 (CX(I, J), J=1,8)

DO 935 I=1, JDN

WRITE(6,934) NSDNBS(I)

FORMAT(1X,8F5.1)

NDIMX=650

NDX=NDIM

IF(NDIM.GT.NDIMX) NDX=NDIMX

DO 10 K=1,8

MDIM(K)=0

DO 10 J=1,NDX

NWEIT1(J,K)=0

DO 10 I=1,8

WEIT(K,J,I)=0.000

NMAX=0

DO 700 IST=1,NDIM

IF(NMAX.EQ.0) GOTO100

DO 20 I=1,NMAX

DO 20 J=1,8

IF(IST.EQ.NWEIT1(I,J)) GOTO 700
CONTINUE
NMAX=NMAX+1
WRITE(6,26) IST
NWEIT1(NMAX,1)=IST
WEIT1(NMAX,1)=1.000
CALL FUD(IST,LU,LD,JDN)
WRITE(6,931) IST,LU,LD
931 FORMAT(1X,5I5)
DO 110 J=1,NSITE
NUP(J)=NSUP(LU,J)
110 NDN(J)=NSDN(LD,J)
FORMAT(1X,814,4X,814)
FORMAT(1X,' INITIAL STATE IS',I9)
FORMAT(1X,'FINAL STATE IS',I9,3X,I9)
DO 2120 IPR=1,3
CALL ROTXYP(IPR, NUP, MUPF, RS)
CALL ROTXYP(IPR, NDN, MDNF, RS1)
NU=INVERT(NSITE, MUPF, RS)
ND=INVERT(NSITE, MDNF)
L=(LOCATE(JUP, NSUPBS, NU)-1)*JDN+LOCATE(JDN, NSDNBS, ND)
WRITE(6,36)IPR,L
NWEIT1(NMAX,IPR+1)=L
WEIT1(NMAX,IPR+1)=RS*RS1
932 GOTO(1010,1020,2120),IPR
1010 DO 120 J=1,NSITE
NUP1(J)=MUPF(J)
120 NDN1(J)=MDNF(J)
CALL ROTXYP(3,NUP1,MUPF, RS)
CALL ROTXYP(3,NDN1,MDNF,RS1)
NU=INVERT(NSITE, MUPF)
ND=INVERT(NSITE, MDNF)
L=(LOCATE(JUP, NSUPBS,NU)-1)*JDN+LOCATE(JDN, NSDNBS, ND)
WRITE(6,36)IPR,L
NWEIT1(NMAX,IPR+1)=L
WEIT1(NMAX,IPR+1)=RS*RS1*WEIT1(NMAX,2)
GOTO(1010,1020,2120),IPR
1020 DO 120 J=1,NSITE
NUP1(J)=MUPF(J)
120 NDN1(J)=MDNF(J)
CALL ROTXYP(3,NUP1,MUPF, RS)
CALL ROTXYP(3,NDN1,MDNF,RS1)
NU=INVERT(NSITE, MUPF)
ND=INVERT(NSITE, MDNF)
L=(LOCATE(JUP, NSUPBS,NU)-1)*JDN+LOCATE(JDN, NSDNBS, ND)
NWEIT1(NMAX,6)=L
WEIT1(NMAX,6)=RS*RS1*WEIT1(NMAX,2)
CALL ROTXYP(2,NUP1,MUPF, RS)
CALL ROTXYP(2,NDN1,MDNF,RS1)
NU=INVERT(NSITE, MUPF)
ND=INVERT(NSITE, MDNF)
L=(LOCATE(JUP, NSUPBS,NU)-1)*JDN+LOCATE(JDN, NSDNBS, ND)
NWEIT1(NMAX,5)=L
WEIT1(NMAX,5)=RS*RS1*WEIT1(NMAX,2)
DO 130 I=1,8
113

NUP1(I) = MUPF(I)
NDN1(I) = MDNF(I)
CALL ROTXYP(3, NUP1, MUPF, RS)
CALL ROTXYP(3, NDN1, MDNF, RS1)
NU = INVERT(NSITE, MUPF)
ND = INVERT(NSITE, MDNF)
L = (LOCATE(JUP, NSUPBS, NU) - 1) * JDN + LOCATE(JDN, NSDNBS, ND)
NWEIT1(NMAX, 8) = L
WEIT1(NMAX, 8) = RS * RS1 * WEIT1(NMAX, 5)
GOTO 2120

1020 DO 140 J = 1, NSITE
NUP1(J) = MUPF(J)
140 WDW1(J) = MDNF(J)
CALL ROTXYP(3, NUP1, MUPF, RS)
CALL ROTXYP(3, NDN1, MDNF, RS1)
NU = INVERT(NSITE, MUPF)
ND = INVERT(NSITE, MDNF)
L = (LOCATE(JUP, NSUPBS, NU) - 1) * JDN + LOCATE(JDN, NSDNBS, ND)
NWEIT1(NMAX, 7) = L
WEIT1(NMAX, 7) = RS * RS1 * WEIT1(NMAX, 3)
CONTINUE

12 FORMAT(1X, 8I8, 4X, 'HAS BEEN USED')
822 FORMAT(1X, 8F8.1, 4X, 'ARE THE SIGN')
C WRITEC6,12)(NWEIT1(NMAX,K),K=1,8)
C WRITE(6,822)(WEIT1(NMAX,K),K=1,8)
700 CONTINUE

738 IF(NMAX.LE.NDIMX) GOTO 2499
739 WRITE(6,2498) NMAX, NDIMX
2498 FORMAT(IX, 'THE DIM OF SUB IS', 19, 'WHICH IS LARGER THAN', 19, 'I9')
STOP
2499 DO 2500 IST = 1, NMAX
2500 I = IST, 1, 8
2501 WS(I) = WEIT1(IST, I)
2510 NS(I) = NWEIT1(IST, I)
DO 800 IXYP = 1, 8
800 NSMAX = MDIM(IXYP)
DO 2501 I = 1, 8
2501 WCS(I) = CX(IXYP, I)
CALL CHECKS(NSITE, WS, NS, WFS, NFS, WCS, ISUM)
IF(ISUM.EQ.0) GOTO 800
DO 2520 I = 1, NMAX
2520 J = I, 8
IF((WFS(J).NE.WEIT(IXYP,1,J)).OR.(NFS(J).NE.NWEIT(IXYP,1,J))
1G0T02520
2521 CONTINUE
2520 CONTINUE
MDIM(IXYP)=MDIM(IXYP)+1
NSHAX=NSMAX+1
DO 2522 J=1,8
WEIT(IXYP,NSHAX,J)=WFS(J)
800 CONTINUE
2500 CONTINUE
C WRITE(6,4)
C4 FORMAT(IX,' IN THE SUB SYBASE')
DO 2025 IXYP=1,8
NDIM1=MDIM(IXYP)
DO 2025 I=1,NDIM1
WRITE(6,2026) (WEIT(IXYP,I,J),J=1,8)
WRITE(6,2027) (NWEIT(IXYP,I,J),J=1,8)
2026 FORMAT(IX,' WEIGHT=',8F8.2)
2027 FORMAT(IX,' STATE=',818)
2025 CONTINUE
1000 RETURN
END
NOTE: THIS PROGRAM APPLY ROTATION OPERATORS TO THE ONE OF THE
BASIS STATES AND GIVE OUT THE RESULT
SUBROUTINE ROTXYP(IPR,NI,NF,S)
IMPLICIT REAL*8(A-H,0-Z)
DIMENSION NI(8),NF(8),NF1(8)
S=1.0D0
GOTO (200,100,300),IPR
100 NF(1)=NI(8)
NF(8)=NI(1)
DO 10 I=1,8
IF(I.EQ.1.0R.I.EQ.8)GOT010
NF(I)=NI(I)
11 NF1(I)=NF(I)
S=S*S1
DO 11 I=1,8
NF2(I)=NF1(I)
11 NF2(I)=NF1(I)
NF(2)=NF1(7)
796   NF(7)=NF(2)
797   DO 12 I=1,8
798   IF(I.EQ.2.OR.I.EQ.7)G0T012
799   NF(I)=NF1(I)
800  12 CONTINUE
801   CALL RSIGN(S1,2,7,NF,8)
802   S=S*S1
803   DO 13 I=1,8
804  13 NF1(I)=NF(I)
805   NF(3)=NF1(6)
806   NF(6)=NF1(3)
807   DO 14 I=1,8
808  14 IF(I.EQ.3.OR.I.EQ.6)G0T014
809   NF(I)=NF1(I)
810  14 CONTINUE
811   CALL RSIGN(S1,3,6,NF,8)
812   S=S*S1
813   DO 15 I=1,8
814  15 NF1(I)=NF(I)
815   NF(4)=NF1(5)
816   NF(5)=NF1(4)
817   DO 16 I=1,8
818  16 IF(I.EQ.4.OR.I.EQ.5)G0T016
819   NF(I)=NF1(I)
820  16 CONTINUE
821   CALL RSIGN(S1,4,5,NF,8)
822   S=S*S1
823   GOTO 500
824  200 NF(1)=NI(6)
825   NF(6)=NI(1)
826   DO 210 I=1,8
827  210 IF(I.EQ.1.OR.I.EQ.6)G0T0210
828   NF(I)=NI(I)
829  210 CONTINUE
830   CALL RSIGN(S1,1,6,NF,8)
831   S=S*S1
832   DO 211 I=1,8
833  211 NF1(I)=NF(I)
834   NF(2)=NF1(5)
835   NF(5)=NF1(2)
836   DO 212 I=1,8
837  212 IF(I.EQ.2.OR.I.EQ.5)G0T0212
838 \( NF(I) = NF1(I) \)
839 212 CONTINUE
840 CALL RSIGN(S1,2,5,NF,8)
841 S=S*S1
842 DO 213 I=1,8
843 213 NF1(I)=NF(I)
844 NF(3)=NF1(8)
845 NF(8)=NF1(3)
846 DO 214 I=1,8
847 IF(I.EQ.3.0R.I.EQ.8)GOTO 214
848 NF(I)=NF1(I)
849 214 CONTINUE
850 CALL RSIGN(S1,3,8,NF,8)
851 S=S*S1
852 DO 215 I=1,8
853 215 NF1(I)=NF(I)
854 NF(4)=NF1(7)
855 NF(7)=NF1(4)
856 DO 216 I=1,8
857 IF(I.EQ.4.0R.I.EQ.7)GOTO 216
858 NF(I)=NF1(I)
859 216 CONTINUE
860 CALL RSIGN(S1,4,7,NF,8)
861 S=S*S1
862 GOTO 500
863 300 NF(1)=NI(7)
864 NF(7)=NI(1)
865 DO 310 I=1,8
866 IF(I.EQ.1.0R.I.EQ.7)GOTO 310
867 NF(I)=NI(I)
868 310 CONTINUE
869 CALL RSIGN(S1,1,7,NF,8)
870 S=S*S1
871 DO 311 I=1,8
872 311 NF1(I)=NF(I)
873 NF(2)=NF1(8)
874 NF(8)=NF1(2)
875 DO 312 I=1,8
876 IF(I.EQ.2.0R.I.EQ.8)GOTO 312
877 NF(I)=NF1(I)
878 312 CONTINUE
879 CALL RSIGN(S1,2,8,NF,8)
117

S=S*S1
DO 313 I=1,8
NF1(I)=NF(I)
NF(3)=NF1(5)
NF(5)=NF1(3)
DO 314 I=1,8
IF(I.EQ.3.OR.I.EQ.5)GOTO 314
NF(I)=NF1(I)
CONTINUE
CALL RSIGN(S1,3,5,NF,8)
S=S*S1
DO 315 I=1,8
NF1(I)=NF(I)
NF(4)=NF1(6)
NF(6)=NF1(4)
DO 316 I=1,8
IF(I.EQ.4.OR.I.EQ.6)GOTO 316
NF(I)=NF1(I)
CONTINUE
CALL RSIGN(S1,4,6,NF,8)
S=S*S1
500 RETURN
END
SUBROUTINE RSIGN(S1,3,5,NF,8)
IMPLICIT REAL*(A-H,0-Z)
DIMENSION NS(NM)
L=NS(I1)+NS(I2)-1
IF(L)10,20,30
S=1.0D0
GOTO 1000
30 S=-1.0D0
GOTO 1000
20 S=1.0D0
I11=MIN0(I1,I2)+1
I22=MAX0(I1,I2)-1
DO 40 I=I11,I22
IF(NS(I).EQ.1) S=-S
40 CONTINUE
1000 RETURN
END

C NOTE: THIS PROGRAM WILL ADD THE STATES OF A CLASS UP TO FORM
C SYMMETRIZED STATES
SUBROUTINE CHECKS(NSTATE,W1,N1,W2,WSCX,ISUM)
IMPLICIT REAL*8(A-H,0-Z)
DIMENSION N1(NSTATE),W2(NSTATE),N2(NSTATE)
DIMENSION NNST(8),WSCX(8),W1(8)
DO 11 I=1,NSTATE
  W2(I)=0.0D0
  N2(I)=0
  NDS=0
  DO 10 I=1,NSTATE
    IF(NDS.EQ.0)GOTO100
    IF(N1(I).EQ.0)GOTO10
    DO 20 J=1,NDS
      IF(N1(I).EQ.NNST(J)) GOTO 10
    20 CONTINUE
  100 NDS=NDS+1
  10 CONTINUE
  NDS1=NDS-1
  DO 500 I=1,NDS1
    I=I+1
    DO 450 J=I1,NDS,1
      IF(NNST(I).LT.NNST(J)) GOTO 450
      L=NNST(I)
      NNST(I)=NNST(J)
      NNST(J)=L
    450 CONTINUE
  500 CONTINUE
  DO 600 I=1,NSTATE
    L=NNST(I)
    DO 610 J=1,NSTATE
      IF(N1(J).NE.L) GOTO 610
      W2(I)=W2(I)+W1(J)*WSCX(J)
      N2(I)=L
    610 CONTINUE
  600 CONTINUE
  WRITE(6,601)(WSUM(I),I=1,NS2)
  WRITE(6,602)(NWSUM(I),I=1,NS2)
  601 FORMAT(1X,10F10.3)
  602 FORMAT(1X,10110)
  IF(W2(1).NE.0.0DO) GOTO 700
DO 630 I=1,NDS
   IF(W2(I).EQ.0.0D0)GOTO 630
   IL=I
   ISUM=1
   GOTO 605
   630 CONTINUE

   ISUM=0
   GOTO 1000

   650 DO 640 1=1,NDS
      L=IL+I-1
      IF(IL.GT.NDS) GOTO 645
      W2(I)=W2(L)
      N2(I)=N2(L)
   640 CONTINUE

   645 W2(I)=0.0D0
   N2(I)=0

   640 CONTINUE

   700 ISUH=1
   SIGN=W2(1)
   SIGN=W2(1)/DABS(SIGN)
   SUM=0.0D0
   DO 710 1=1,NDS
      SUM=SUM+W2(I)*W2(I)
   710 SUM=DSQRT(SUM)
   DO 720 1=1,NDS
      W2(I)=SIGN*W2(I)/SUM
   720 W2(I)=SIGN*W2(I)/SUM
   1000 RETURN

END

SUBROUTINE FUD(L,LU,LD,JDN)
   LD=MOD(L,JDN)
   IF(LD.EQ.0) LD=JDN
   LU=(L-LD)/JDN+1
   RETURN
END

SUBROUTINE GENLST(NEL,NSITE,JQ,NSV)
   CALL GENLST(NEL,NSITE,JUP,NSUP)

   DIMENSION NSTV(100,8)
   JQ=1
   IF(NSITE.EQ.8)GO TO 1
   WRITE(6,100)
   100 FORMAT(1X,'FATAL ERROR, INCORRECT NUMBER OF SITES IN GENLST')
   STOP
CONTINUE
DO 1000 I=1,100
DO 1000 J=1,NSITE
1000 NSTV(I,J)=0
IF(NEL.LE.0)RETURN
JQ=0
DO 10 N1=1,2
DO 9 N2=1,2
DO 8 N3=1,2
DO 7 N4=1,2
DO 6 N5=1,2
DO 5 N6=1,2
DO 4 N7=1,2
DO 3 N8=1,2
1020 IF(N1+N2+N3+N4+N5+N6+N7+N8.NEL+NSITE)GO TO 3
1021 JQ=JQ+1
1022 NSTV(JQ,1)=N1-1
1023 NSTV(JQ,2)=N2-1
1024 NSTV(JQ,3)=N3-1
1025 NSTV(JQ,4)=N4-1
1026 NSTV(JQ,5)=N5-1
1027 NSTV(JQ,6)=N6-1
1028 NSTV(JQ,7)=N7-1
1029 NSTV(JQ,8)=N8-1
3 CONTINUE
4 CONTINUE
5 CONTINUE
6 CONTINUE
7 CONTINUE
8 CONTINUE
9 CONTINUE
10 CONTINUE
RETURN
END
SUBROUTINE SIGN(SGN, NTL, NVR, M1,M2,IV)
IMPLICIT REAL*8(A-H,O-Z)
DIMENSION NVR(100,8)
SGN=1.0D0
IF(NTL.EQ.0)RETURN
MA=MAX0(M1,M2)
MB=MIN0(M1,M2)
IF(MA-MB.NE.1)GO TO 1
1048 RETURN
1049 1 IF(MA-MB.GT.2)GO TO 2
1050 MC=MB+1
1051 IF(NVR(IV,MC).GT.0)SGN=-1.0
1052 RETURN
1053 2 MC=MA-1
1054 MD=MB+1
1055 NSUM=0
1056 DO 3 IX=MD,MC
1057 IF(NVR(IV,IX).GT.0)NSUM=NSUM+1
1058 3 CONTINUE
1059 SGN=(-1.0)**NSUM
1060 RETURN
1061 END
1062 CCCCCCCCCCCC
1063 C ----------------------------------------------------------
1064 C TO CONVERT THE A BASIS STATE TO BINARY SEARCHABLE NUMBER
1065 FUNCTION INVERT(NSITE,NOS)
1066 DIMENSION NOS(NSITE)
1067 INVERT=0
1068 DO 100 I=1,NSITE
1069 100 INVERT=INVERT+N0S(I)*10**(NSITE-I)
1070 300 RETURN
1071 END
1072 C TO CONVERT THE A SET BASIS STATE TO BINARY SEARCHABLE NUMBERS
1073 SUBROUTINE TRANS(NDIM, NSITE, NOS, NFS)
1074 C C
1075 CALL TRANS(JUP,NSITE,NSUP,NSUPBS) ---------
1076 DIMENSION NOS(100,8),NFS(100)
1077 IF(NSITE.NE.8) GOTO 200
1078 DO 100 I=1,NDIM
1079 100 NSUM=0
1080 DO 50 J=1,NSITE
1081 50 CONTINUE
1082 NFS(I)=NSUM
1083 100 CONTINUE
1084 GOTO 300
1085 200 WRITE(6,1)
1086 STOP
1087 1 FORMAT(IX,'THE FATAL ERROR THE NSITE IS WRONG IN THE SUB TRANS')
1088 300 RETURN
1089 END
SUBROUTINE SIGN1(NVR, NS, II, SGN)
IMPLICIT REAL*8(A-H, O-Z)
DIMENSION NVR(NS)
SGN=1.0D0
IF(II.EQ.1)RETURN
ND=II-1
NSUM=0
DO 3 IX=1,ND
IF(NVR(IX).GT.0)NSUM=NSUM+1
3 CONTINUE
SGN=(-1.0)**NSUM
RETURN
END

SUBROUTINE SIGN2(NVR, II, SGN, I)
IMPLICIT REAL*8(A-H, O-Z)
DIMENSION NVR(100, 8)
SGN=1.0D0
IF(II.EQ.1)RETURN
ND=II-1
NSUM=0
DO 3 IX=1,ND
IF(NVR(I, IX).GT.0)NSUM=NSUM+1
3 CONTINUE
SGN=(-1.0)**NSUM
RETURN
END

C---- PROCESS DC(C,D) ----

SUBROUTINE SPEFC(JUP1, JDN1, JUP2, JDN2, NSITE,
INUP, NDIM1, NDIM2, JQ1, JQ2, NK, NSUP1, NSDN1, NSUP2, NSDN2)

C PROGRAM TO OBTAIN THE QUANTUM EXPECTATION OF OPERATOR:
C(K,+,IS)
C NOTE: +,- DENOTING RAISING AND LOWERING OP. ;
C * K INDEXES OF WAVE VECTOR;
C * IS,JS SPIN ; IS=1 FOR UP, WHILE IS=-1 FOR DOWN;
C * NSUP1(NDIM,NSITE) & NSDN1 ARE THE ARRAYS TO STORE
C THE BASIS STATES OF N ELECTRON SYSTEM;
C * NSUP2 & NSDN2 ARE BASIS STATES OF N+1 ELECTRON SYSTEM;
C * NSUPBS & NSDNBS ARE THE BASIS STATES CONVERTED TO NUMBERS
C AND TO BE USED IN BINARY SEARCH;
* PH(K,ISITE) ARE PHASE FACTORS;
NPOP(I,J) = <I|OPERATOR(J)|K> * K
CIDN(NK,I,J) ARE THE OUTPUT OF QUANTUM
EXPECTATION VALUE: <I|G(NK,-,IS=1)|J>

IMPLICIT REAL*8(A-H,O-Z)
DIMENSION NSUP1(100,8),NSDN1(100,8),NSUP2(100,8),NSDN2(100,8)
DIMENSION NSUPBS(100),NSDNSBS(100),PH(8,4)
DIMENSION NUP2(58),NDN2(58),NSIGN(58),WKK(5000,650,8)
DIMENSION NPOP(5000,8),WK(5000,650,4)
DIMENSION ZDUM1(650,5000),ZDUM2(650,5000),CIDN(4,650,650)
COMMON /C/ZDUM1,ZDUM2,CIDN/D/WKK, WK
DATA PH/1.DO,1.DO,1.DO,1.DO,1.DO,1.DO,1.DO,1.DO,
 * 1.DO,-1.DO,-1.DO,1.DO,1.DO,1.DO,1.DO,1.DO,
 * 1.DO,-1.DO,1.DO,-1.DO,1.DO,-1.DO,1.DO,-1.DO,
 * 1.DO,-1.DO,1.DO,-1.DO,1.DO,-1.DO,1.DO,-1.DO/
WRITE(6,*)' SUBROUTINE INPUT'
WRITE(6,*)NSITE
NDIM=0
DO 99 I1=1,JUP1
DO 99 J1=1,JDN1
NDIM=NDIM+1
WRITE(6,89)NDIM,(NSUP1(I1,I),1=1,NSITE)
WRITE(6,89)NDIM,(NSDN1(I,J1),1=1,NSITE)
NDIM=0
DO 29 12=1,JUP2
DO 29 J2=1,JDN2
NDIM=NDIM+1
WRITE(6,89)NDIM,(NSUP2(I2,I),1=1,NSITE)
WRITE(6,89)NDIM,(NSDN2(J2,I),1=1,NSITE)
DO 39 1=1,JQ1
39 WRITE(6,*)' ZDUM1',(ZDUM1(I,J),J=1,NDIM1)
IF(JUP1.EQ.8.AND.JDN1.EQ.1) THEN
DO 40 I=1,JQ2
40 WRITE(6,*)' ZDUM2',(ZDUM2(I,J),J=1,NDIM2)
ENDIF
WRITE (  6,89) JUP1, JDN1,  JUP2,  JDN2,  NSITE
WRITE(6,89)NUP, NDIM1,NDIM2,JQ1,JQ2,NK
WRITE(6,*)' END OF THE SUB INPUT'
WRITE(6,101) LSTMX, NDIMX, NDIM, NPRMX, NPR
DO 3232 K=1,NK
3232 WRITE(6,323)(PH(I,K),1=1,NSITE)
ISPIN=-1
DO 11 J=1,NSITE
DO 11 I=1,NDIM22
NPOP(I,J)=0
DO 12 I=1,NSITE
DO 12 J=1,JQ1
WKK(J,I,II)=0.DO
GET THE BINARY SEARCH BASIS READY, I.E., CONVERT THE BASIS STATES
TO A SERIES OF NUMBERS
***
CALL TRANS(JUP1,NSITE,NSUP1,NSUPBS)
CALL TRANS(JDN1,NSITE,NSDN1,NSDNBS)
DO 1000 I=1,NSITE
NSUM=0
DO 500 ISU=1,JUP2
DO 700 ISD=1,JDN2
NSUM=NSUM+1
NI=NSUP2(ISU,II)*((ISPIN+1)/2)+NSDN2(ISD,II)*((-ISPIN)/2)
IF(NI.NE.1) GOTO 700
DO 550 I=1,NSITE
NUP2(I)=NSUP2(ISU,I)
550  NDN2(I)=NSDN2(ISD,I)
DO 590 I=1,NSITE
NSIGN(I)=NUP2(I)*((ISPIN+1)/2)+NDN2(I)*((-ISPIN)/2)
CALL SIGN1(NSIGN,NSITE,II,SI)
IF(ISPIN) 591,591,592
591  NDN2(II)=0
592  NUP2(II)=0
593  CONTINUE
WRITE(6,553)
FORMAT(1X,'THE FINAL STATE IS')
WRITE(6,99) (NUP2(I),I=1,NSITE),(NDN2(I),I=1,NSITE)
FIND OUT WHICH STATE THE RESULTING STATE IS
NUP2BS=INVERT(NSITE,NUP2)
NDN2BS=INVERT(NSITE,NDN2)
WRITE(6,554) NUP2BS,NDN2BS
FORMAT(1X,'THE BS FOR FINAL STATE IS',4I4)
LUP=LOCATE(JUP1,NSUPBS,NUP2BS)
1216  LDN=LOCATE(JDN1,NSDNBS,NDN2BS)
1217  L=(LUP-1)*JDN1+LDN
1218  IF(SI.LT.0.0D0)L=-L
1219  IF(ISPIN.EQ.-1) L=L*(-1)**NUP
1220  NPOP(NSUM,II)=L
1221  WRITE(6,89) LUP,LDN,L
1222  700  CONTINUE
1223  500  CONTINUE
1224  DO 900 JQ=1,JQ1
1225  DO 800 IJ=1,NDIM22
1226  J=NPOP(IJ,II)
1227  IF(J.NE.0) THEN
1228  SN=1.0
1229  IF(J.LT.0) THEN
1230  J = - J
1231  SN=-SN
1232  ENDIF
1233  C WKK(IJ,JQ,II)=WKK(IJ,JQ,II)+SN
1234  ENDIF
1235  800  CONTINUE
1236  900  CONTINUE
1237  86  WRITE(6,*)II,IJ,(WKK(IJ,JQ,II),JQ=1,JQ1)
1238  C ENDIF
1239  1000 CONTINUE
1240  DO 134 K=1,NK
1241  DO 134 JQ=I,JQI
1242  DO 134 IJ=1,NDIM22
1243  WK(IJ,JQ,K)=0.D0
1244  DO 134 K=1,NK
1245  DO 135 I=1,NSITE
1246  DO 135 JQ=I,JQI
1247  DO 135 IJ=1,NDIM22
1248  WK(IJ,JQ,K)=WK(IJ,JQ,K)+WKK(IJ,JQ,II)*PH(II,K)
1249  IF(JUP1.EQ.8.AND.JDN1.EQ.1) THEN
1250  WRITE(6,*)' DEVIDE'
1251  DO 87 I=1,NDIM22
1252  WRITE(6,*)K,IJ,(WK(IJ,JQ,1),JQ=1,JQ1)
1253  C ENDIF
DO 77 K=1,NK
DO 77 IQ=1,JQ1
DO 77 JQ=1,JQ2
CIDN(K,IQ,JQ)=0.D0
DO 88 JQ=1,JQ2
DO 88 IQ=1,JQ1
DO 88 K=1,NK
DO 85 MN=1,NDIM22
CIDN(K,IQ,JQ)=CIDN(K,IQ,JQ)+WK(MN,IQ,K)*ZDUM2(JQ,MN)
CONTINUE
CIDN(K,IQ,JQ)=CIDN(K,IQ,JQ)/DSQRT(DFLOAT(NSITE))
CONTINUE
DO 111 IK=1,NK
DO 111 IQ=1,JQ1
WRITE(6,*)(*CIDN(IK,IQ,JQ),JQ=1,JQ2)
9999 RETURN
197 ^197 END
FUNCTION LOCATE(IDIM,IMAT,IVAL)
LOCATE FINDS THE INDEX FOR WHICH IMAT(LOCATE)=IVAL.
LOCATE IS ASSIGNED ZERO IF IMAT DOES NOT CONTAIN IVAL.
NOTE: IMAT ENTRIES MUST BE IN INCREASING ORDER.
NO DUPLICATE ENTRIES ARE ALLOWED IN IMAT.
DIMENSION IMAT(IDIM)
MID=0
MIN=1
MAX=IDIM+1
LOCATE=(MIN+MAX)/2
IF(LOCATE.EQ.MID)GO TO 40
MID=LOCATE
IF(IMAT(LOCATE)-IVAL)30,50,20
MAX=LOCATE
GO TO 10
MIN=LOCATE
GO TO 10
LOCATE=0
50 RETURN
END
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//♦0.FT16F001 DD DSN=PHTANL.HUB7E(U6),UNIT=DISK,DISP=SHR
//♦0.FT21F001 DD DSN=PHTANL.GKV1(GR6),UNIT=DISK,DISP=SHR
//♦0.FT22F001 DD DSN=PHTANL.GKV2(GR6),UNIT=DISK,DISP=SHR
//♦0.FT23F001 DD DSN=PHTANL.GKV3(GR6),UNIT=DISK,DISP=SHR
//♦0.FT24F001 DD DSN=PHTANL.GKV4(GR6),UNIT=DISK,DISP=SHR
//♦0.SYSIN DD *

1  2
1 2 NRTL
1  2 NPR
2  3
3  4
4  1
5  6
6  7
7  8
8  5
1  5
2  6
3  7
4  8
5  1
6  2
7  3
8  4

U

NTHOP THOPIN DTHOP

NTLIN NTLFL

B T

ELIM9 YSC9

ELIM7 YSC7

HWIN DW

D NK

EMINT
A.2 Conductivity

1 //PHTANL1 JOB (1103,69869,220,22),'PHTANL',MSGLEVEL=(1,1),
2 // MSGCLASS=S,CLASS=H
3 /*JOBPARM SHIFT=D
4 /*AFTER GBC812
5 /*ROUTE PRINT RNT4
6 //S1 EXEC VSF2CLG,REGION.F0RT=2560K,
7 // PARM.F0RT='SOURCE,NOTERM,OPT(3),VEC',
8 // PARM.LKED='NOMAP,NOXREF,LIST,LET,AMODE=ANY',
9 // PARM.GO='NOXUFL0W',
10 // REGION.GO=99M,TIME.GO=999,
11 // LIB='SY51.ESVVLIB'
12 //FORT.SYSIN DD *
13 @PROCESS DC(Y)
14 C-------------------------------------------------------------
15 C FOLLOWING PROGRAM TO PERFORM HUBBARD MODEL CALCULATION FOR
16 C CUBIC CLUSTER BY MEANS OF SYMMETRIZED BASIS AND CALCULATE
17 C THE ELECTRIC CONDUCTIVITY.
18 C NSITE=# OF SITES; NTL=# OF TOTAL ELECTRONS
19 C NPRTL=TOTAL NUMBER OF NEAREST NEIGHBOR PAIRS
20 C UIN IS PARAMETER IN HUBBARD MODEL; THOP IS T
21 C EIGENENERGIES ARE STORED IN EN ARRAY
22 NOTE:
23 C MIJX ARE OPERATOR PAIRS
24 C D IS THE WIDTH PARAMETER
25 C RESULTS ARE STORED IN FILE CONDT
26 C-------------------------------------------------------------
27 C IMPLICIT REAL*8(A-H,O-Z)
28 COMPLEX*16 D1,D2
29 DIMENSION WK(1300),ZDUM(5000),EN(5000)
30 DIMENSION WEIT(8,650,8),NWEIT(8,650,8),MDIM(8)
31 DIMENSION HWV(211575),ENW(650),ZDUMW(650,650),ZGRD(7,5000)
32 DIMENSION NSUP(100,8),NSDN(100,8),NPR(50,2),NDIF1(8),NDIF2(8)
33 DIMENSION NUIMIN(10),ND1MIN(10),PH(8,8)
34 DIMENSION NME(10),EL(10),WX1(5000,8),WX2(5000,8)
35 DIMENSION WX(5000,8),WXB(5000,8)
36 DIMENSION NSUPBS(100),NSDNSBS(100),DITG(8)
37 DIMENSION MIJ(3,16),JV(5000,16),CXX(8,1000),DX(8,1000)
38 DIMENSION RCXX(8,8,1000),SUM(8),SUMX(8,8),TA(8),EK(8),EKA(8)
DIMENSION DK1(8,8,1000),DK2(8,8,1000)

COMMON /C/JV

COMMON /C1/NSUP,NSDN

COMMON /C2/NSUPBS,NSDNSBS,JUP,JDN

COMMON /C3/NPR,NUP,NDN,NSITE,NPRTL

COMMON /Y/HWV,ZDUMW

DATA PH/ 1.DO,1.DO,1.DO,1.DO,1.DO,1.DO,1.DO,1.DO,
* 1.DO,-1.DO,-1.DO,1.DO,1.DO,-1.DO,-1.DO,1.DO,
* 1.DO,-1.DO,1.DO,-1.DO,1.DO,-1.DO,-1.DO,1.DO,
* 1.DO,-1.DO,1.DO,-1.DO,1.DO,-1.DO,1.DO,-1.DO,
* 1.DO,1.DO,-1.DO,1.DO,1.DO,-1.DO,-1.DO,1.DO,
* 1.DO,1.DO,1.DO,1.DO,-1.DO,-1.DO,-1.DO,1.DO,
* 1.DO,-1.DO,-1.DO,1.DO,-1.DO,1.DO,-1.DO,-1.DO,
* 1.DO,1.DO,-1.DO,-1.DO,-1.DO,-1.DO,1.DO,-1.DO,
* 1.DO,1.DO,-1.DO,-1.DO,1.DO,1.DO,1.DO,-1.DO,
* 1.DO,1.DO,1.DO,1.DO,-1.DO,-1.DO,-1.DO,1.DO/

CALL ERRSET(208,0,-1,0,1,1)

C==========================================================
C DEFINE SYSTEM
NDIMX=650
NDIMX2=2*NDIMX
NSITE=8
PI=3.1415926

C ----------- THIS PARAMETER MUST AGREE WITH # OF SITES ----
C PARAMETER NDIMX MUST AGREE WITH DIMENSION OF HW
C ----------- CHECK THE PARAMETERS ABOVE ----------------

C ----------------------READ IN DATA----------------------
READ(5,100)NPRTL
WRITE(6,100)
DO 1 I=1,NPRTL
  READ(5,102)NPR(I,1),NPR(I,2)
1 CONTINUE
102 FORMAT(2I5)
READ(5,101)U
READ(5,106)NTHQP,THOPIN,DTHOP
READ(5,102)NTLIN,NTLFL
READ(5,*)NW,WIN,DW1
READ(5,*)ICUT,W2,DW2
C WRITE(6,*)NW,WIN,DW
C READ(5,*)NK,D
READ(5,*)NPRMX
DO 3140 I=1,NPRMX
  READ(5,*)(MIJ(K,I),K=1,3)
3140 CONTINUE
3140 READ(5,*)(MIJ(K,I),K=1,3)
NCORMX=30
LSTMX=100
DO 9999 NTL=NTLIN,NTLFL
THOP=THOPIN
IF(NTL-NSITE)1000,1000,1001
1000 NUPST=NTL+1
NMMAX=NTL
GO TO 1002
1001 NUPST=NSITE+1
NMMAX=2*NSITE-NTL
1002 DO 310 IU=1,NTH0P
WRITE(6,6788) NTL
WRITE(16,6788) NTL
WRITE(6,6789)U,THOP
WRITE(16,6789)U,THOP
WRITE(6,6791)
6791 FORMAT(IX,' THE ENERGY UNIT IS T IN HUBBARD MODEL/)
6788 FORMAT(IX,' THE FOLLOWING RESULTS ARE ABOUT CUBIC CLUSTER WITH
   \* ',14,' ELECTRONS ')
6789 FORMAT(IX,' HUBBARD MODEL CALCULATION WHEN U=',F10.4,5X,' T=',
   \* F10.4,5X)
6614 FORMAT(IX,' T VS S-C-FN. U,THOP=',2F6.2)
10483 FORMAT(IX, F 
   \* F6.2,4X, F 
   \* F6.2)
114 FORMAT(IX,' EIGENENERGIES ARE FOLLOWING: ')
106 C --------------PERFORM CALCULATION IN DIFFERENT Sz SUBSPACES ------------
IRC=0
DO 300 IRAN=1,NTL
NUP=NUPST-IRAN
IF(NUP.LE.0)GO TO 301
NDN=NTL-NUP
IF(NDN.GT.NUP)GO TO 301
100 FORMAT(I5)
101 FORMAT(F10.5)
IRANMX=IRAN
C ------------------ GENERATE BASIS FUNCTIONS ---------------------
CALL GENLST(NUP,NSITE,JUP,NSUP)
CALL GENLST(NDN,NSITE,JDN,NSDN)
C ----------------------------------------------------------------
NDIM=JUP*JDN
WRITE(16,103)NUP,JUP, NDN, JDN, NDIM, NSITE
WRITE(6,103)NUP,JUP, NDN, JDN, NDIM, NSITE
124 103 FORMAT(1X,'NUP,JUP,NDN,JDN,NDIM,NSITE=','15I5)
125 C FIND THE ATOMIC SPINS ON EACH SITE
126 C IF(THOP.NE.0.01DO) GOTO 200
127 C JQ=0
128 C DO 200 IA=1,JUP
129 C DO 200 IB=1,JDN
130 C JQ=JQ+1
131 C ================ IT'S HERE ==============================
132 C 200 WRITE(6,104)JQ,(NSUP(IA,K),K=1,NSITE),(NSDN(IB,K),K=1,NSITE)
133 C 104 FORMAT(18,3X,813,3X,813)
134 DO 2001 IQXY=1,NDIM
135 2001 EN(IQXY)=0.0DO
136 C -----------------CONVERT BASIS TO BINARY CODE -----------------
137 CALL TRANS(JUP,NSITE,NSUP,NSUPBS)
138 CALL TRANS(JDN,NSITE,NSDN,NSDNBS)
139 C -----------------CONSTRUCT SYMMETRIZED BASIS -----------------
140 CALL SYBASE(WEIT,NWEIT,MDIM,NSITE,NDIM)
141 C ------------GENERATE MATRIX ELEMENTS BETWEEN BASIS FUNCTIONS ---
142 CALL CIJ(NSUP,NSDN,NSUPBS,NSDNBS,JUP,JDN,NSITE,LSTMX,
143 1 5000,NDIM,MIJ,NPRMX)
144 C DO 543 J=1,NPRMX
145 C 543 WRITE(6,778)(JV(I,J),1=1,NDIM)
146 C 778 FORMAT(2813)
147 2021 FORMAT(IX,' THE DIM OF SYMMETRIZED STATES ARE',219)
148 EMIN1=1000.D0
149 C ---------------------------------------------
150 DO 542 NAD=1,2
151 C JQ=0
152 C JQ=1
153 C =========== BEGIN TO GENERATE HAMILTONIAN ============
154 DO 7777 IXYP=1,8
155 C NDM1=MDIM(IXYP)
156 C WRITE(6,2021)IXYP,NDIM1
157 C NDM2=NDIM1*(NDIM1+1)/2
158 IF(NDIM1.EQ.0) GOTO7777
159 DO 9100 I=1,NDIM1
160 ENW(I)=0.0DO
161 DO 9100 J=1,NDIM1
162 9100 ZDUMW(I,J)=0.0DO
163 DO 9113 I=1,NDM2
164 9113 HWV(I)=0.0DO
165 IAB=0
DO 9230 IA=1,NDIM1
DO 9230 JB=IA,NDIM1
IAB=IAB+1
DO 9220 I=1,8
II=NWEIT(IXYP,IA,I)
IF(II.EQ.0) GO TO 9220
DO 9221 J=1,8
JJ=NWEIT(IXYP,JB,J)
IF(JJ.EQ.0) GO TO 9221
X=HIAB(II,JJ,JDW,U,THOP)
HWV(IAB)=HWV(IAB)+WEIT(IXYP,IA,I)*WEIT(IXYP,JB,J)*X
CONTINUE
CONTINUE
CONTINUE
CONTINUE
C==================================================================================================
C 3859 FORMAT(1X,'THE HAMILTONIAN IS follows')
C ---DIAGONALIZE HAMILTONIAN----------------------
CALL EIGRS(HWV, NDIM1,2,ENW, ZDUMW, NDIMX, WK,IER)
CALL DSLEV(1,HWV, ENW,ZDUMW, NDIMX, NDIM1, WK,NDIMX2)
C Store eigenenergies and wavefunctions -----------
DO 7830 I=1,NDIM1
JQ=JQ+1
EN(JQ)=ENW(I)
WRITE(6,*)EN(JQ)
DO 9101 J=1,NDIM
DO 7820 J=1,NDIM1
DO 7820 K=1,8
MN=NWEIT(IXYP, J,K)
IF(MN.EQ.0) GO TO 7820
ZDUM(MN)=ZDUM(MN)+WEIT(IXYP,J,K)*ZDUMW(J,I)
CONTINUE
CONTINUE
IF(NAD.EQ.1) THEN
IF((EN(JQ)-EMIN1).LT.1.0D-12) THEN
IF(DABS(EN(JQ)-EMIN1).LT.1.0D-12) THEN
JQG=JQG+1
ELSE
JQG=1
ENDIF
ENDIF
ENDIF
EMIN1=EN(JQ)
DO 911 M=1,NDIM
ZGRD(JQG,M)=ZDUM(M)
208      JQGMAX=JQG
209      ENDIF
210 C     WRITE(6,231)JJ,JQ,(ZDUM(IZ),IZ=1,NDIM)
211 C231  FORMAT(2I5,8F8.3)
212      GOTO 7830
213 ELSEIF(NAD.EQ.2) THEN
214 C     WRITE(6,*)(NSITE,NK,NPRMX,NDIM,JQ,JQGMAX
215 C     WRITE(6,231)(ZDUM(IZ),IZ=1,12)
216 C231  FORMAT(12F8.4)
217 C     WRITE(6,*)(MIJ(I,IPR),IPR=1,NPRMX)
218 C8 98 WRITE(6,654) (MIJ(I,IPR),IPR=1,NPRMX)
219 C654  FORMAT(1X,20I5)
220      C ----------------BEGIN GENERATING MATRIX ELEMENTS-------------------
221      DO 242 K=1,NK
222      WKX(A(JQ,K)=0.DO
223 C242  WKXB(JQ,K)=0.DO
224      TA(IRAN)=0.DO
225      DO 3012 JJ=1,JQGMAX
226      DO 241 K=1,NK
227      WKX1(JQ,K)=0.D0
228 C241  WKX2(JQ,K)=0.D0
229      DO 3010 II=1,NDIM
230      ISITE=M1J(2,IPR)
231      J=JV(II,IPR)
232      IF(J.NE.0) THEN
233      SN=1.DO
234      IF(J.LT.0) THEN
235      J=-J
236      SN=-SN
237      END IF
238      SN=SN
239      END IF
240      IF(IPR.GT.NPRMX/2) SN=-SN
241      DO 909 K=1,NK
242      WKX1(JQ,K)=WKX1(JQ,K)+SN*ZDUM(J)*ZGRD(JJ,II)*PH(ISITE,K)
243      WKX2(JQ,K)=WKX2(JQ,K)+SN*ZDUM(II)*ZGRD(JJ,J)*PH(ISITE,K)
244 909  END IF
245      TA(IRAN)=TA(IRAN)+THOP*SM*ZGRD(JJ,J)*ZGRD(JJ,II)/DFLOAT(JQGMAX)
246      221 CONTINUE
247      3010 CONTINUE
248      DO 908 K=1,NK
\[ WKXA(jq,K) = WKXA(jq,K) + DABS(WKX1(jq,K))^{2}/DFLOAT(JQMAX) \]

\[ WKXB(jq,K) = WKXB(jq,K) + DABS(WKX2(jq,K))^{2}/DFLOAT(JQMAX) \]

901 CONTINUE

3012 CONTINUE

901 CONTINUE

3754 FORMAT(1X,' K,JQ,EN,WKXA,WKXB',215,8F8.3)

ENDIF

7777 CONTINUE

542 CONTINUE

WRITE(6,*)' KE',EMIN1,TA(IRAN)

C DO 4321 JJ=1,JQGMAX

C WRITE(6,231)JJ,CZGRDCIZ,JJ),IZ=1,NDIM)

C DO 4323 JQ=1,NDIM

C WRITE(6,3754)EN(JQ),(WKX1(JQ,K),K=1,NK)

C4323 WRITE(6,3754)EN(JQ),(WKX2(JQ,K),K=1,NK)

C3754 FORMAT(1X,F8.4,5E16.5)

C OUTPUT EIGENENERGIES

-----------------------

5432 WRITE(6,6601)

WRITE(16,6601)

DO 7790 I=1,NDIM,5

I4=I+4

IF(I4.GT.NDIM) I4=NDIM

WRITE(6,105)I,(EN(KI),KI=I,14)

WRITE(16,105)I,(EN(KI),KI=I,I4)

7790 CONTINUE

105 FORMAT(I5,15E20.8)

6601 FORMAT(1X,' THE EIGENENERGIES ARE')

----------------------- FINISH OUTPUT EIGENENERGIES -----------------------

C FIND THE MIN ENERGY IN THE SUBSPACE ---------------------

EMIN=EN(1)

NMIN=1

NME(1)=1

IF (NDIM.EQ.1) GOTO 3701

DO 3700 IXY=2,NDIM

IF (DABS(EMIN-EN(IXY)).LT.1.0D-12) GOTO 3721

IF (EMIN.LT.EN(IXY)) GOTO 3700

EMIN=EN(IXY)

NMIN=1

NME(1)=IXY
292    GOTO 3700
293  3721  NMIN=NMIN+1
294    NME(NMIN)=IXY
295  3700  CONTINUE
296  3701  NU1MIN(IRAN)=NUP
297    ND1MIN(IRAN)=NDN
298    EL(IRAN)=EMIN
299    WRITE(6,3021)EMIN,(NME(NXY),NXY=1,NMIN)
300  3021  FORMAT(1X,' THE GROUND STATE IS EN,K',E15.6,10I5)
301  3022  FORMAT(8E15.6)
302    EP=0.0D0
303    DO 6543 JJ=1,JQGMAX
304      JQE=0
305    DO 6543 IE=1,JUP
306      DO 6543 JE=1,JDN
307        JQE=JQE+1
308    DO 6542 ISITE=1,NSITE
309  6542  EP=EP+U*DFLOAT(NSUP(IE,ISITE))*DFLOAT(NSDN(JE,ISITE))
310      *ZGRD(JJ,JQE)**2/DFLOAT(JQGMAX)
311  6543  CONTINUE
312    EK(IRAN)=EMIN-EP
313    EKA(IRAN)=EK(IRAN)/3.0D0
314    C END OF EMIN ; BEGINNING OF CALCULATING CONDUCTIVITY ---------
315  177  FORMAT(1X,I4,F8.4,4E16.5)
316    AM=0.5D0*DFLOAT(NUP-NDN)
317    L=NDN/NUP
318    L=1+1/(1+L)
319    X1=DFLOAT(L)
320    W=WIN
321    DW=DW1
322    DO 98 I=1,NW
323      DO 324 K=1,NK
324        CXX(K,I)=0.0D0
325      DXX(K,I)=0.0D0
326    SUM(K)=0.0D0
327  324  CONTINUE
328    DSFM=0.0D0
329    DO 95 JQ=1,NDIM
330      RDE1=W+EMIN-EN(JQ)
331      RDE2=W-EMIN+EN(JQ)
332      D1=DCMPLX(RDE1,D)
333      D2=DCMPLX(RDE2,D)
DO 435 K=1,NK
AXX=WXXA(JQ,K)
BXX=WXXB(JQ,K)
CXX(K,I)=CXX(K,I)-DIMAG(AXX/D1-BXX/D2)/W
DXX(K,I)=DXX(K,I)+DREAL(AXX/D1-BXX/D2)
IF(ABS(EMIN-EN(JQ)).LT.1.0D-12) GOTO 435
DE=EMIN-EN(JQ)
SUM(K)=SUM(K)-PI*(AXX+BXX)/DE/2.DO
435 CONTINUE
95 CONTINUE
WRITE(6,*) 'SUM',(SUM(K),K=1,NK)
XM=GAM*AM
IF(NUP.EQ.NDN) GO TO 97
DO 3031 K=1,NK
RCXX(K,IRAN,I)=CXX(K,I)
DK1(K,IRAN,I)=1.DO-4.DO*PI*(DXX(K,I)-EKA(IRAN))/W**2
DK2(K,IRAN,I)=4.DO*PI*CXX(K,I)/W
SUMX(K,IRAN)=SUM(K)
3031 CONTINUE
GO TO 98
IF(I.EQ.ICUT) THEN
W=W2
DW=DW2
ENDIF
98 W=W+DW
IRC=IRC+1
WRITE(6,301) ' THE TOTAL POSSIBLE CONFIGURATION OF NUP&NDN IS',I4,3X,'IRANMX=',I4
301 NMIN=1
EMIN=EL(1)
WRITE(6,3134) IRC,IRANMX
DO 299 IRAN=1,IRANMX
IF(EL(IRAN).GE.EMIN) GO TO 299
EMIN=EL(IRAN)
NMIN=IRAN
299 CONTINUE
DO 3710 IY=1,IRC
WRITE(6,3711) EL(IY),NUIMIN(IY),ND1MIN(IY)
3711 FORMAT(1X,'THE POSSIBLE MIN ENERGY IS ',E20.5,' WHEN NUP=',I4,3X,'N
*DN=',I4)
WRITE(6,111)EMIN,NU1MIN(NMIN),ND1MIN(NMIN)

111 FORMAT(1X,'THE MIM ENERGY IS',E20.5,'WHEN NUP=',I4,3X,'NDN=',I4)

W=W1
DW=DW1

C WRITE(6,162)U,NTL
C WRITE(22,162)U,NTL

162 FORMAT(1X,'REAL PART OF DIEL. FUN. FOLLOW U=',F8.4,2X,'N=',I5)
DO 3510 I=1,NW
C WRITE(6,3531)I,W,(DK1(K,NMIN,I),K=1,NK)
C WRITE(22,3531)I,W,(DK1(K,NMIN,I),K=1,NK)

C -----------------------BEGIN OUTPUT -------------------------------

IF(I.EQ.ICUT) THEN

W=W2
DW=DW2
ENDIF

3510 W=W+DW
W=W1
DW=DW1

C WRITE(6,152)U,NTL
C WRITE(24,152)U,NTL

152 FORMAT(1X,'IMAG. PART OF DIEL. FUN. FOLLOW U=',F8.4,2X,'N=',I5)
DO 3520 I=1,NW
C WRITE(6,3532)I,W,(DK2(K,NMIN,I),K=1,NK)
C WRITE(24,3532)I,W,(DK2(K,NMIN,I),K=1,NK)

IF(I.EQ.ICUT) THEN

W=W2
DW=DW2
ENDIF

3520 W=W+DW

WRITE(6,112)U,NTL
WRITE(26,112)U,NTL

112 FORMAT(1X,'OPTICAL CONDUCTIVITY FOLLOW U=',F8.4,2X,'N=',I5)
W=W1
DW=DW1

DO 658 K=1,NK

658 DITG(K)=0.DO
DO 3533 I=1,NW

DO 659 K=1,NK

IF(I.EQ.1) GOTO 659
RX1=RCXX(K,NMIN,I-1)
RX2=RCXX(K,NMIN,I)

DITG(K)=DITG(K)+(RX1+RX2)*DW/2.DO
CONTINUE
WRITE(26,3531)I,W,(RCXX(K,NMIN,I),K=1,NK)
C WRITE(6,3531)I,W,(RCXX(K,NMIN,I),K=1,NK)
IF(I.EQ.ICUT) THEN
  W=W2
  DW=DW2
ENDIF
3533 W=W+DW
C WRITE(6,3538) (SUMX(K,NMIN),K=1,NK)
WRITE(26,3538) (SUMX(K,NMIN),K=1,NK)
WRITE(6,3539) (DITG(K),K=1,NK)
DRU=-PI*EKA(NMIN)-2.DO*SUMX(1,NMIN)
C WRITE(6,*),'DRUDE=',DRU
C WRITE(26,*),'KEA=',EKA(NMIN)
FORMAT(1X,15,2X,F10.4,20E13.5)
3531 FORMAT(1X,I5,2X,F10.4,20E13.5)
3538 FORMAT(1X,'SUM',14X,20E13.5)
3539 FORMAT(1X,'INT',14X,20E13.5)
310 THOP=THOP+DTHOP
9999 CONTINUE
WRITE(6,115)
WRITE(26,115)
115 FORMAT(1X,'END OF DATA. ')
STOP
END
C THIS FUNCTION GIVE THE <IA|H|IB> FOR PARAMETER U,T IN THE H
FUNCTION HIAB(IA,IB,JDN,U,T)
IMPLICIT REAL*(A-H,0-Z)
DIMENSION NSUP(100,8),NSDN(100,8),NPR(50,2),NDIF1(8),NDIF2(8)
COMMON /C1/NSUP,NSDN
COMMON /C3/NPR,NUP,NDN,NSITE,NPRTL
333 HIAB=0.0DO
CALL FUD(IA,IAU,IAD,JDN)
CALL FUD(IB,IBU,IBD,JDN)
IF(IA.NE.IB) GOTO 20
IF(NDN.EQ.0) GO TO 999
DO 10 I=1,NSITE
  IF(NSUP(IAU,I).EQ.1.AND.NSDN(IAD,I).EQ.1) HIAB=HIAB+U
10 CONTINUE
GOTO 999
DO 30 I=1,NSITE
   NDIF1(I)=NSUP(IAU,I)-NSUP(IBU,I)
   NDIF2(I)=NSDN(IAD,I)-NSDN(IBD,I)
   ISUM1=ISUM1+NDIF1(I)
   ISUM2=ISUM2+NDIF2(I)
   ISUM3=ISUM3+IABS(NDIF1(I))
   ISUM4=ISUM4+IABS(NDIF2(I))
30 CONTINUE
IF(ISUM3.GT.2) GO TO 999
IF(ISUM4.GT.2) GO TO 999
IF(ISUM1.NE.0) GO TO 999
IF(ISUM2.NE.0) GO TO 999
IF(ISUM3.EQ.2.AND.ISUM4.EQ.2) GO TO 999
C ONE MOVE HAS OCCURRED. IS IT A NEAREST NEIGHBOR PAIR?
IF(ISUM3.EQ.0) GO TO 100
MUS1=0
MUS2=0
MX=0
DO 40 ME=1,NSITE
   MX=MX+1
   IF(MUS1.NE.0) GO TO 45
   IF(NDIF1(ME).NE.0) MUS1=MX
40 CONTINUE
IF(NDIF1(ME).NE.0) GO TO 41
45 IF(NDIF1(ME).NE.0) GO TO 41
40 CONTINUE
GO TO 999
41 MUS2=MX
IPRU=0
DO 50 MF=1,NPRTL
   IX=NPR(MF,1)-MUS1
   IY=NPR(MF,2)-MUS2
   IF(IX.NE.0) GO TO 55
   IF(IY.NE.0) GO TO 55
   IPRU=1
50 CONTINUE
GO TO 51
55 IX=NPR(MF,1)-MUS2
500 IY=NPR(MF,2)-MUS1
501 IF(IX.NE.0) GO TO 50
140

IF(IY.NE.0)GO TO 50
503  IPRU=1
504  GO TO 51
505  50 CONTINUE
506  IF(IPRU.NE.1)GO TO 999
507  51 CALL SIGN(SGN,NUP,NSUP,MUS1,MUS2,IAU)
508  GO TO 998
509  100 MDS1=0
510  IF(NDN.EQ.0)GO TO 999
511  MX=0
512  MDS2=0
513  DO 145 ME=1,NSITE
514   MX=MX+1
515  IF(MDS1.NE.0)GO TO 140
516  IF(NDIF2(ME).NE.0)MDS1=MX
517  GO TO 145
518  140 IF(NDIF2(ME).NE.0)GO TO 146
519  145 CONTINUE
520  GO TO 999
521  146 MDS2=MX
522  IPRD=0
523  DO 155 MF=1,NPRTL
524    IX=NPR(MF,1)-MDS1
525    IY=NPR(MF,2)-MDS2
526  IF(IX.NE.0)GO TO 150
527  IF(IY.NE.0)GO TO 150
528  IPRD=1
529  GO TO 151
530  150 IX=NPR(MF,1)-MDS2
531    IY=NPR(MF,2)-MDS1
532  IF(IX.NE.0)GO TO 155
533  IF(IY.NE.0)GO TO 155
534  IPRD=1
535  GO TO 151
536  155 CONTINUE
537  IF(IPRD.NE.1)GO TO 999
538  151 CALL SIGN(SGN,NDN,NSDN,MDS1,MDS2,IAD)
539  998 HIAB=T*SGN
540  999 RETURN
541 END

C NOTE: THIS PROGRAM TO SYMMETRIZE A SET OF BASIS
542 SUBROUTINE SYBASE(WEIT,NWEIT,MDIM,NSITE,NDIM)
544 IMPLICIT REAL*8(A-H,0-Z)
545 DIMENSION WEIT(8,650,8),NWEIT(8,650,8),CX(8,8)
546 DIMENSION NWEIT(650,8),NSUPBS(100),NSDNBS(100)
547 DIMENSION WEIT(650,8)
548 DIMENSION NSUP(100,8),NSDN(100,8),MDIM(8)
549 DIMENSION NSUSED(100),NUP(8),NDN(8),NUP1(8),NDN1(8)
550 DIMENSION WS(8),NS(8),WFS(8),NFS(8),NSUM(8),NSUM1(8),WSUM(8)
551 DIMENSION MUPF(8),MDNF(8),WCS(8)
552 COMMON /C1/NSUP,NSDN
553 COMMON /C2/NSUPBS,NSDNBS,JUP,JDN
554 DATA CX/1.0D0,1.0D0,1.0D0,1.0D0,1.0D0,1.0D0,1.0D0,1.0D0,1.0D0,1.0D0,1.0D0,1.0D0,1.0D0,-1.0D0,-1.0D0,-1.0D0,-1.0D0,-1.0D0,-1.0D0,-1.0D0,1.0D0,1.0D0,-1.0D0,-1.0D0,1.0D0,1.0D0,-1.0D0,-1.0D0,-1.0D0,-1.0D0,1.0D0,-1.0D0,1.0D0,-1.0D0,1.0D0,-1.0D0,-1.0D0,1.0D0,-1.0D0,-1.0D0,1.0D0,-1.0D0,-1.0D0,1.0D0,-1.0D0,-1.0D0,1.0D0,-1.0D0,-1.0D0,1.0D0/-
555 C DO 933 1=1,8
556 C933 WRITE(6,934)(CX(I,J),J=1,8)
557 NDIMX=650
558 NDX=NDIM
559 IF(NDIM.GT.NDIMX) NDX=NDIMX
560 DO 10 K = 1,8
561 MDIM(K)=0
562 DO 10 J=1,NDX
563 NWEIT1(J,K)=0
564 DO 10 I=1,8
565 WEIT(K,J,I)=0.0D0
566 10 NWEIT(K,J,I)=0
567 NMAX=0
568 DO 700 IST=1,NDIM
569 IF(NMAX.EQ.0) GOTO100
570 DD 20 I=1,NMAX
571 DD 20 J=1,8
572 IF(IST.EQ.NWEIT1(I,J)) GOTO 700
573 CONTINUE
574 NMAX=NMAX+1
575 WRITE(6,26) IST
586     NWEIT1(NMAX,1)=IST
587     WEIT1(NMAX,1)=1.0D0
588     CALL FUD(IST,LU,LD,JDN)
589     C     WRITE(6,931) IST,LU,LD
590     931   FORMAT(1X,5I5)
591     DO 110 J=1,NSITE
592     NUP(J)=NSUP(LU,J)
593  110    NDN(J)=NSDN(LD,J)
594     21   FORMAT(1X,8I4,4X,8I4)
595     26   FORMAT(1X,'INITIAL STATE IS',I9)
596     36   FORMAT(1X,'FINAL STATE IS',I9,3X,I9)
597     DO 2120 IPR=1,3
598     CALL ROTXY(I,PR,IPR,NUP,MUPF,RS)
599     CALL ROTXY(IPR,NDN,MDNF,RS1)
600     NU=INVERT(NSITE,MUPF,RS)
601     ND=INVERT(NSITE,MDNF)
602     L=(LOCATE(JUP,NSUPBS,NU)-1)*JDN+LOCATE(JDN,NSDNBS,ND)
603     C     WRITE(6,36)IPR,L
604     NWEIT1(NMAX,IPR+1)=L
605     WEIT1(NMAX,IPR+1)=RS*RS1
606     932   G0T0(1010,1020,2120),IPR
607  1010   DO 120 J=1,NSITE
608     NUP1(J)=MUPF(J)
609  120    NDN1(J)=MDNF(J)
610     CALL ROTXY(I,PR,3,NUP1,MUPF,RS)
611     CALL ROTXY(3,NDN1,MDNF,RS1)
612     NU=INVERT(NSITE,MUPF)
613     ND=INVERT(NSITE,MDNF)
614     L=(LOCATE(JUP,NSUPBS,NU)-1)*JDN+LOCATE(JDN,NSDNBS,ND)
615     NWEIT1(NMAX,6)=L
616     WEIT1(NMAX,6)=RS*RS1*WEIT1(NMAX,2)
617     CALL ROTXY(2,NUP1,MUPF,RS)
618     CALL ROTXY(2,NDN1,MDNF,RS1)
619     NU=INVERT(NSITE,MUPF)
620     ND=INVERT(NSITE,MDNF)
621     L=(LOCATE(JUP,NSUPBS,NU)-1)*JDN+LOCATE(JDN,NSDNBS,ND)
622     NWEIT1(NMAX,5)=L
623     WEIT1(NMAX,5)=RS*RS1*WEIT1(NMAX,2)
624     DO 130 I=1,8
625     NUP(I)=MUPF(I)
626  130    NDN(I)=MDNF(I)
627     CALL ROTXY(3,NUP1,MUPF,RS)
CALL ROTXYP(3,NDN,MDNF,RSI)

NU=INVERT(NSITE,MUPF)

ND=INVERT(NSITE,MDNF)

L=(LOCATE(JUP,NSUPBS,NU)-1)*JDN+LOCATE(JDN,NSDNBS,ND)

NWEIT(NMAX,8)=L

WEIT(NMAX,8)=RS*RSI*WEIT(NMAX,5)

GOTO 2120

1020 DO 140 J=1,NSITE

NUP(J)=MUPF(J)

140 NDN(J)=MDNF(J)

CALL ROTXYP(3,NUP1,MUPF,RS)

CALL ROTXYP(3,NDN1,MDNF,RSI)

NU=INVERT(NSITE,MUPF)

ND=INVERT(NSITE,MDNF)

L=(LOCATE(JUP,NSUPBS,NU)-1)*JDN+LOCATE(JDN,NSDNBS,ND)

NWEIT(NMAX,7)=L

WEIT(NMAX,7)=RS*RSI*WEIT(NMAX,3)

2120 CONTINUE

12 FORMAT(IX,8I8,4X,'HAS BEEN USED')

822 FORMAT(IX,8F8.1,4X,'ARE THE SIGN')

WRITE(6,12)(NWEIT(NMAX,K),K=1,8)

WRITE(6,822)(WEIT(NMAX,K),K=1,8)

700 CONTINUE

IF(NMAX.LE.NDIMX) GOTO 2499

WRITE(6,2498)NMAX,NDIMX

2498 FORMAT(IX,' THE DIM OF SUB IS ',19,' WHICH IS LARGER THAN',19)

STOP

2499 DO 2500 IST=1,NMAX

DO 2510 I=1,8

WS(I)=WEIT1(IST,I)

2510 NS(I)=NWEIT1(IST,I)

DO 800 IXYP=1,8

NSMAX=MDIM(IXYP)

DO 2501 I=1,8

2501 WCS(I)=CX(IXYP,I)

DO 2520 J=1,8

IF((WFS(J).NE.WEIT(IXYP,I,J)) .OR. (NFS(J).NE.NWEIT(IXYP,I,J)))

GOTO 2520

2521 CONTINUE
GOTO 2500
2520 CONTINUE
MDIM(IXYP) = MDIM(IXYP) + 1
NSMAX = NSMAX + 1
DO 2522 J = 1, 8
   WEIT(IXYP, NSMAX, J) = WFS(J)
   NWEIT(IXYP, NSMAX, J) = NFS(J)
2522 CONTINUE
800 CONTINUE
2500 CONTINUE
C WRITE(6, 4)
   FORHAT(1X, 'IN THE SUB SYBASE')
DO 2025 IXYP = 1, 8
   NDIM1 = MDIM(IXYP)
DO 2025 I = 1, NDIM1
   WRITE(6, 2026) (WEIT(IXYP, I, J), J = 1, 8)
   WRITE(6, 2027) (NWEIT(IXYP, I, J), J = 1, 8)
2026 FORMAT(IX, ' WEIGHT=', 8F8.2)
2027 FORMAT(IX, ' STATE=', 8I8)
2025 CONTINUE
1000 RETURN
END
C NOTE: THIS PROGRAM APPLY ROTATION OPERATORS TO THE ONE OF THE
BASIS STATES AND GIVE OUT THE RESULT
SUBROUTINE ROTXYP(IPR, NI, NF, S)
IMPLICIT REAL*8(A-H,O-Z)
DIMENSION NI(8), NF(8), NF1(8)
S = 1.0D0
GOTO (200, 100, 300), IPR
100 NF(1) = NI(8)
   NF(8) = NI(1)
   DO 10 I = 1, 8
      IF(I .EQ. 1.0R1.EQ. 8) GOTO 10
      NF(I) = NI(I)
   10 CONTINUE
   CALL RSIGN(S1, 1, 8, NF, 8)
   S = S * S1
   DO 11 I = 1, 8
      IF(I .EQ. 1.0R1.EQ. 7) GOTO 11
      NF1(I) = NF(I)
      NF(2) = NF1(7)
      NF(7) = NF1(2)
   11 DO 12 I = 1, 8
      IF(I .EQ. 2.0R1.EQ. 7) GOTO 12
      NF1(I) = NF(I)
   12 CONTINUE
712   NF(I)=NF1(I)
713   12 CONTINUE
714   CALL RSIGN(S1,2,7,NF,8)
715   S=S*S1
716   DO 13 I=1,8
717   13   NF1(I)=NF(I)
718   NF(3)=NF1(6)
719   NF(6)=NF1(3)
720   DO 14 I=1,8
721   IF(I.EQ.3.0R.I.EQ.6)G0T014
722   NF(I)=NF1(I)
723   14 CONTINUE
724   CALL RSIGN(S1,3,6,NF,8)
725   S=S*S1
726   DO 15 I=1,8
727   15 NF1(I)=NF(I)
728   NF(4)=NF1(5)
729   NF(5)=NF1(4)
730   DO 16 I=1,8
731   IF(I.EQ.4.0R.I.EQ.5)G0T016
732   NF(I)=NF1(I)
733   16 CONTINUE
734   CALL RSIGN(S1,4,5,NF,8)
735   S=S*S1
736   GOTO 500
737   200 NF(1)=NI(6)
738   NF(6)=NI(1)
739   DO 210 I=1,8
740   IF(I.EQ.1.0R.I.EQ.6)G0T0210
741   NF(I)=NI(I)
742   210 CONTINUE
743   CALL RSIGN(S1,1,6,NF,8)
744   S=S*S1
745   DO 211 I=1,8
746   211 NF1(I)=NF(I)
747   NF(2)=NF1(5)
748   NF(5)=NF1(2)
749   DO 212 I=1,8
750   IF(I.EQ.2.0R.I.EQ.5)G0T0212
751   NF(I)=NF1(I)
752   212 CONTINUE
753   CALL RSIGN(S1,2,5,NF,8)
S=S*S1
DO 213 I=1,8
  NF1(I)=NF(I)
  NF(3)=NF1(8)
  NF(8)=NF1(3)
  DO 214 I=1,8
    IF(I.EQ.3.0R.I.EQ.8)GOTO 214
    NF(I)=NF1(I)
  214 CONTINUE
  CALL RSIGN(S1,3,8,NF,8)
  S=S*S1
DO 215 I=1,8
  NF1(I)=NF(I)
  NF(4)=NF1(7)
  NF(7)=NF1(4)
  DO 216 I=1,8
    IF(I.EQ.4.0R.I.EQ.7)GOTO 216
    NF(I)=NF1(I)
  216 CONTINUE
  CALL RSIGN(S1,4,7,NF,8)
  S=S*S1
  GOTO 500
300 NF(1)=NI(7)
  NF(7)=NI(1)
  DO 310 I=1,8
    IF(I.EQ.1.0R.I.EQ.7)GOTO 310
    NF(I)=NI(I)
  310 CONTINUE
  CALL RSIGN(S1,1,7,NF,8)
  S=S*S1
DO 311 I=1,8
  NF1(I)=NF(I)
  NF(2)=NF1(8)
  NF(8)=NF1(2)
  DO 312 I=1,8
    IF(I.EQ.2.0R.I.EQ.8)GOTO 312
    NF(I)=NF1(I)
  312 CONTINUE
  CALL RSIGN(S1,2,8,NF,8)
  S=S*S1
DO 313 I=1,8
  NF1(I)=NF(I)
796    NF(3)=NF1(5)
797    NF(5)=NF1(3)
798    DO 314 I=1,8
799    IF(I.EQ.3.OR.I.EQ.5)GOTO 314
800    NF(I)=NF1(I)
801  314 CONTINUE
802    CALL RSIGN(S1,3,5,NF,8)
803    S=S*S1
804    DO 315 I=1,8
805  315 NF1(I)=NF(I)
806    NF(4)=NF1(6)
807    NF(6)=NF1(4)
808    DO 316 I=1,8
809    IF(I.EQ.4.OR.I.EQ.6)GOTO 316
810    NF(I)=NF1(I)
811  316 CONTINUE
812    CALL RSIGN(S1,4,6,NF,8)
813    S=S*S1
814  500 RETURN
815  END
816  SUBROUTINE RSIGN(S1,I1,I2,NS,NM)
817  IMPLICIT REAL*8(A-H,0-Z)
818  DIMENSION NS(NM)
819    L=NS(I1)+NS(I2)-1
820  10 IF(L)10,20,30
821   10 S=1.0D0
822   20 GOTO 1000
823   30 S=-1.0D0
824   40 GOTO 1000
825   50 S=1.0D0
826    I11=MIN0(I1,I2)+1
827    I22=MAX0(I1,I2)-1
828    DO 40 I=I11,I22
829    IF(NS(I).EQ.1) S=-S
830  40 CONTINUE
831  1000 RETURN
832  END
833  C NOTE: THIS PROGRAM WILL ADD THE STATES OF A CLASS UP TO FORM
834  C SYMMETRIZED STATES
835  SUBROUTINE CHECKS(NSTATE,W1,N1,W2,N2,WSCX,ISUM)
836  IMPLICIT REAL*8(A-H,0-Z)
837  DIMENSION N1(NSTATE),W2(NSTATE),N2(NSTATE)
148

DIMENSION NNST(8),WSCX(8),W1(8)
DO 11 I=1,NSTATE
W2(I)=0.0D0
11 N2(I)=0
NDS=0
DO 10 I=1,NSTATE
IF(NDS.EQ.0)GOTO100
IF(N1(I).EQ.0)GOTO10
DO 20 J=1,NDS
IF(N1(I).EQ.NNST(J)) GOTO 10
20 CONTINUE
NDS=NDS+1
NNST(NDS)=N1(I)
10 CONTINUE
13 FORMAT(IX,' THE DIFF STATES ARE ',815)
310 NDS1=NDS-1
DO 500 1=1,NDS1
11=1+1
DO 450 J=I1,NDS,1
IF(NNST(I).LT.NNST(J))  GOTO 450
L=NNST(I)
NNST(I)=NNST(J)
NNST(J)=L
450 CONTINUE
500 CONTINUE
DO 600 1=1,NDS
L=NNST(I)
DO 610 J=1,NSTATE
IF(NKJ).NE.L) GOTO 610
W2(I)=W2(I)+W1(J)*WSCX(J)
N2(I)=L
610 CONTINUE
600 CONTINUE
WRITE(6,601)(WSUM(I),I=1,NS2)
WRITE(6,602)(NHSUM(I),1=1,NS2)
601 FORMAT(IX,10F10.3)
602 F0RMAT(1X,10110)
CC NORMALIZATION AND LET WSUM(I) LARGER THAN ZERO
IF(W2(I).NE.0.0D0) GOTO 700
DO 630 I=1,NDS
IF(W2(I).EQ.0.0D0)GOTO 630
IL=I
ISUM=1
GOTO 650
CONTINUE
ISUM=0
GOTO 1000
DO 640 I=1,NDS
L=IL+I-1
IF(IL.GT.NDS) GOTO 645
W2(I)=W2(L)
N2(I)=N2(L)
GOTO 640
W2(I)=0.0D0
N2(I)=0
CONTINUE
ISUM=1
SIGN=W2(1)
SIGN=H2(1)/DABS(SIGN)
SUM=0.0D0
DO 710 I=1,NDS
SUM=SUM+W2(I)*W2(I)
SUM=DSQRT(SUM)
DO 720 I=1,NDS
W2(I)=SIGN*W2(I)/SUM
1000 RETURN
END
SUBROUTINE FUD(L,LU,LD,JDN)
LD=MOD(L,JDN)
IF(LD.EQ.0) LD=JDN
LU=(L-LD)/JDN+1
RETURN
END
SUBROUTINE GENLST(NEL,NSITE,JQ,NSTV)
DIMENSION NSTV(100,8)
JQ=1
IF(NSITE.EQ.8) GOTO 1
WRITE(6,100)
100 FORMAT(1X,'FATAL ERROR, INCORRECT NUMBER OF SITES IN GENLST')
STOP
CONTINUE
DO 1000 I=1,100
DO 1000 J=1,NSITE
NSTV(I,J)=0
150
922 IF(NEL.EQ.0)RETURN
923 JQ=0
924 DO 10 N1=1,2
925 DO 9 N2=1,2
926 DO 8 N3=1,2
927 DO 7 N4=1,2
928 DO 6 N5=1,2
929 DO 5 N6=1,2
930 DO 4 N7=1,2
931 DO 3 N8=1,2
932 IF(N1+N2+N3+N4+N5+N6+N7+N8.NEL+NSITE)GO TO 3
933 JQ=JQ+1
934 NSTV(JQ,1)=N1-1
935 NSTV(JQ,2)=N2-1
936 NSTV(JQ,3)=N3-1
937 NSTV(JQ,4)=N4-1
938 NSTV(JQ,5)=N5-1
939 NSTV(JQ,6)=N6-1
940 NSTV(JQ,7)=N7-1
941 NSTV(JQ,8)=N8-1
942 3 CONTINUE
943 4 CONTINUE
944 5 CONTINUE
945 6 CONTINUE
946 7 CONTINUE
947 8 CONTINUE
948 9 CONTINUE
949 10 CONTINUE
950 RETURN
951 END
952 SUBROUTINE SIGN(SGN,NTL,NVR,M1,M2,IV)
953 IMPLICIT REAL*8(A-H,0-Z)
954 DIMENSION NVR(100,8)
955 SGN=1.0DO
956 IF(NTL.EQ.1)RETURN
957 MA=MAX0(M1,M2)
958 MB=MIN0(M1,M2)
959 IF(MA-MB.NE.1)GO TO 1
960 RETURN
961 1 IF(MA-MB.GT.2)GO TO 2
962 MC=MB+1
963 IF(NVR(IV,MC).GT.0)SGN=-1.0
RETURN
2 MC=MA-1
MD=MB+1
NSUM=0
DO 3 IX=MD,MC
IF(NVR(IV,IX).GT.0)NSUM=NSUM+1
3 CONTINUE
SGN=(-1.0)**NSUM
RETURN
END

C -------------------------------------------------------------
C TO CONVERT THE A BASIS STATE TO BINARY SEARCHABLE NUMBER
FUNCTION INVERT(NSITE,NOS)
DIMENSION NOS(NSITE)
INVERT=0
DO 100 I=1,NSITE
100 INVERT=INVERT+NOS(I)*10**(NSITE-I)
300 RETURN
END

C TO CONVERT THE A SET BASIS STATE TO BINARY SEARCHABLE NUMBERS
SUBROUTINE TRANS(NDIM,NSITE,NOS,NFS)
C C CALL TRANS(JUP,NSITE,NSUP,NSUPBS)
DIMENSION N0S(100,8),NFS(IOO)
IF(NSITE.NE.8) GOTO 200
DO 100 1=1,NDIM
NSUM=0
DO 50 J=1,NSITE
NSUM=NSUM+NOS(I,J)*10**(NSITE-J)
50 CONTINUE
NFS(I)=NSUM
100 CONTINUE
GOTO 300
200 WRITE(6,1)
STOP
1 FORMAT(IX,'THE FATAL ERROR THE NSITE IS WRONG IN THE SUB TRANS')
300 RETURN
END

SUBROUTINE RSIGN(S,I1,I2,NS,NM)
IMPLICIT REAL*8(A-H,0-Z)
DIMENSION NS(NM)
L=NS(I1)+NS(I2)-1
1006 IF(L) 10,20,30
1007 10 S=1.0D0
1008 GOTO 1000
1009 30 S=-1.0D0
1010 GOTO 1000
1011 20 S=1.0D0
1012 II1=MIN0(I1,I2)+1
1013 I22=MAX0(I1,I2)-1
1014 DO 40 I=II1,I22
1015 IF(NS(I).EQ.1) S=-S
1016 40 CONTINUE
1017 1000 RETURN
1018 END

C-------------------------------
1020 SUBROUTINE CIJ(NSUP,NSDN,NSUPBS,NSDNBS,JUP,JDN,NSITE,LSTMX,
1021 NDIMX,NDIM,MIJ,NPR)
1022 C PROGRAM TO THE QUANTUM EXPECTATION OF OPERATOR:
1023 C C(I,+,IS)*C(J,-,IS)
1024 C NOTE: +,- DENOTING RAISING AND LOWERING OP.;
1025 C * I,J SITE INDEXES;
1026 C * IS SPIN ; IS=1 FOR UP, WHILE IS=-1 FOR DOWN;
1027 C * NSUP(NDIM,NSITE) & NSDN ARE THE ARRAYS TO STORE
1028 C THE BASIS STATES;
1029 C * NSUPBS & NSDNBS ARE THE BASIS STATES CONVERTED TO NUMBERS
1030 C AND TO BE USED IN BINARY SEARCH;
1031 C * MIJ(3,NPRMX) ARRAY TO STORE IJ AND IS;
1032 C * NPR IS # OF THE SETS OF IJ ;
1033 C * NPOP(I,J) = <K 1 OPERATOR(J)|I> * K
1034 C-------------------------------
1035 IMPLICIT REAL*8(A-H,O-Z)
1036 DIMENSION NSUP(LSTMX,1),NSDN(LSTMX,1)
1039 DIMENSION NSUPBS(1),NSDNBS(1)
1040 DIMENSION NUP1(58),NDM1(58),NSIGN(58)
1041 DIMENSION NPOP(5000,16),MIJ(3,1)
1042 COMMON /C/NPOP
1043 C WRITE(6,101) LSTMX,NDIMX,NDIM,NPRMX,NPR
1044 101 FORMAT(IX,' LSTMX,NDIMX,NDIM,NPRMX,NPR=',915)
1045 DO 11 I=1,NDIM
1046 DO 11 J=1,NPR
1047 11 NPOP(I,J)=0
GET THE BINARY SEARCH BASIS READY, I.E., CONVERT THE BASIS STATES TO A SERIES OF NUMBERS

CALL TRANS(JUP, NSITE, NSUP, NSUPBS)
CALL TRANS(JDN, NSITE, NSDN, NSDNBS)
NSUM = 0
DO 520 ISU = 1, JUP
DO 520 ISD = 1, JDN
NSUM = NSUM + 1
520 WRITE(6, 465) NSUM, (NSUP(ISU, J), J = 1, NSITE), (NSDN(ISD, J), J = 1, NSITE)

DO 1000 IPR = 1, NPR
II = MIJ(1, IPR)
JJ = MIJ(2, IPR)
ISPIN = MIJ(3, IPR)
NSUM = 0
DO 500 ISU = 1, JUP
DO 700 ISD = 1, JDN
NSUM = NSUM + 1
NJ = NSUP(ISU, JJ) * ((ISPIN + l)/2) + NSDN(ISD, JJ) * ((1 - ISPIN)/2)
IF(NJ .NE. l) GOTO 700
DO 550 1 = 1, NSITE
NUP1(1) = NSUP(ISU, I)
NDN1(I) = NSDN(ISD, I)
WRITE(6, 551)
FORMAT(1X, 'THE INITIAL STATE IS')
WRITE(6, 89) (NUP1(I), I = 1, NSITE), (NDN1(I), I = 1, NSITE)
89 FORMAT(1X, 11114)
88 FORMAT(1X, 'THE SIGN IS ', F4.0)
DO 560 I = 1, NSITE
560 NSIGN(I) = NUP1(I) * ((ISPIN + l)/2) + NDN1(I) * ((1 - ISPIN)/2)
CALL SIGNK(NSIGN, NSITE, JJ, SJ)
IF(ISPIN) 561, 561, 562
561 NDN1(JJ) = 0
562 NI = NUP1(II) * ((1 + ISPIN)/2) + NDN1(II) * ((1 - ISPIN)/2)
IF(NI. NE. 0) GOTO 700
DO 570 I = 1, NSITE
570 NSIGN(I) = NUP1(I) * ((ISPIN + l)/2) + NDN1(I) * ((1 - ISPIN)/2)
CALL SIGNK(NSIGN, NSITE, II, SI)
IF(ISPIN) 570, 570, 572
571 NDN1(II) = 1
1090   GOTO 573
1091  572  NUP1(II)=1
1092  573  S=SI*SJ
1093  C   WRITE(6,553)
1094  C553  FORMAT(1X,'THE FINAL STATE IS')
1095  C   WRITE(6,554) (NUP1(I),I=1,NSITE),(NDN1(I),I=1,NSITE)
1096  C FIND OUT WHICH STATE THE RESULTING STATE IS
1097     NUP1BS=INVERT(NSITE,NUP1)
1098     NDN1BS=INVERT(NSITE,NDN1)
1099  C   WRITE(6,554) NUP1BS,NDN1BS
1100  554  FORMAT(IX,'THE BS FOR FINAL STATE IS',414)
1101  LUP=LOCATE(JUP,NSUPBS,NUP1BS)
1102  LDN=LOCATE(JDN,NSDNBS,NDN1BS)
1103     L=(LUP-1)*JDN+LDN
1104  IF(S.LT.0.00D0)L=-L
1105  NPOP(NSUM,IPR)=L
1106  CONTINUE
1107  CONTINUE
1108  CONTINUE
1109  9999  RETURN
1110  END
1111  SUBROUTINE SIGN1(NVR,NS,II,SGN)
1112     IMPLICIT REAL*8(A-H,0-Z)
1113     DIMENSION NVR(NS)
1114     SGN=1.0D0
1115  IF(II.EQ.1)RETURN
1116     ND=II-1
1117     NSUM=0
1118  DO 3 IX=1,ND
1119  IF(NVR(IX).GT.0)NSUM=NSUM+1
1120  3 CONTINUE
1121     SGN=(-1.0)**NSUM
1122  RETURN
1123  END
1124  FUNCTION LOCATE(IDIM,IMAT,IVAL)
1125  LOCATE FINDS THE INDEX FOR WHICH IMAT(LOCATE)=IVAL.
1126  LOCATE IS ASSIGNED ZERO IF IMAT DOES NOT CONTAIN IVAL.
1127  NOTE: IMAT ENTRIES MUST BE IN INCREASING ORDER.
DIMENSION IMAT(IDIM)
MIN=0
MAX=IDIM+1

10 LOCATE=(MIN+MAX)/2
IF(LOCATE.EQ.MID)GO TO 40
MID=LOCATE
IF(IMAT(LOCATE)-IVAL)30,50,20
20 MAX=LOCATE
GO TO 10
30 MIN=LOCATE
GO TO 10
40 LOCATE=0
50 RETURN
END

FUNCTION INVERT(NSITE,NOS)
DIMENSION NOS(NSITE)
INVERT=0
DO 100 I=1,NSITE
100 INVERT=INVERT+NOS(I)*2**(NSITE-I)
300 RETURN
END

SUBROUTINE TRANS(NDIM,NSITE,NOS,NFS,LSTMX)
IMPLICIT REAL*8(A-H,O-Z)
DIMENSION NOS(LSTMX,1),NFS(1)
DO 100 I=1,NDIM
NSUM=0
DO 50 J=1,NSITE
NSUM=NSUM+NOS(I,J)*2**(NSITE-J)
50 CONTINUE
NFS(I) = NSUM
100 CONTINUE
IF (NDIM GT 1) THEN
   NDI = NDIM - 1
   DO 400 I = 1, NDI
      I1 = I + 1
      DO 400 J = I1, NDIM
         IF (NFS(J) LT NFS(I)) THEN
            WRITE (6, 2) I, J, NFS(I), NFS(J)
               2 FORMAT (IX, ' THE # IN THE ARRAY MUST BE IN INCREASING ORDER', 416)
      END IF
   400 CONTINUE
END IF
300 RETURN
END

C=================================================================================
//G0.FT16F001 DD DSN=PHTANL.HU8E(U6),UNIT=DISK,DISP=SHR
//G0.FT26F001 DD DSN=PHTANL.CONDT(U6),UNIT=DISK,DISP=SHR
//G0.FT22F001 DD DSN=PHTANL.REALDI(U6),UNIT=DISK,DISP=SHR
//G0.FT24F001 DD DSN=PHTANL.IMAGDI(U6),UNIT=DISK,DISP=SHR
//G0.SYSIN DD *
12 NPRTL
1 2 NPR
2 3
3 4
4 1
5 6
6 7
7 8
8 5
1 5
2 6
3 7
4 8 NPR
6.00 U
1 1.0 0.2 NTHOP THOPIN DTHOP
8 8 NTLIN NTLFL
1000 0.01 0.02 NW WIN DW1
2000 35.0 0.02 ICUT W2 DW2
8 0.05 NK D
16 NPRMX
2 1 1 MIJX
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<td>5</td>
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<tr>
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<td>7</td>
<td>8</td>
<td>1</td>
</tr>
<tr>
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<td>1</td>
<td>-1</td>
</tr>
<tr>
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<td>3</td>
<td>4</td>
<td>-1</td>
</tr>
<tr>
<td>1221</td>
<td>6</td>
<td>5</td>
<td>-1</td>
</tr>
<tr>
<td>1222</td>
<td>7</td>
<td>8</td>
<td>-1</td>
</tr>
<tr>
<td>1223</td>
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VITA

Lun Tan was born on August 26, 1962 in Beijing, China. He received the degree of Bachelor of Science in Physics from Shandong University, China in 1984. He worked in Xian Petroleum Institute as an instructor from 1984 to 1986. In January 1987, he came to the United States for post-graduate studies. He worked under the supervision of Professor Callaway since 1988.
Candidate: Lun Tan

Major Field: Physics

Title of Dissertation: Dynamic Properties of Interacting Electrons

Approved:

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Major Professor and Chairman

Dean of the Graduate School

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May 3, 1993