JUDD OPERATOR METHODS IN SUPERSPACE: APPLICATION TO THE THERMAL SINGLE

PARTICLE GREEN FUNCTION FOR THE HUBBARD DIMER

by

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This manuscript is dedicated to the memory of

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I. INTRODUCTION

In recent years a great deal of literature has been devoted to the metal-insulator transition. The problem of why many solids with narrow partially filled conduction bands are insulating rather than metallic was first studied by Mott[1,2]. The system he investigated was a periodic lattice consisting of atoms with partially filled non-degenerate outer shells (e.g. the 1s shell of hydrogen). Investigation of the electronic properties of such a system usually involves single-electron states in the calculation and electron-electron interactions are taken into account in some self-consistent mean-field manner. In this scheme intra-atomic correlation effects are treated perturbatively. This is the format of band theory calculations. In the context of band theory, the system studied by Mott is a metal. It is easy to see that this description is incomplete as the system remains a metal for any value of the lattice constant. For large enough separations such that each site may be treated as independent, the system ceases to be metallic. It is for intermediate values of the lattice constant that the metal-insulator or "Mott" transition is thought to occur. At this point experimental evidence is still inconclusive. Mott concluded that the failure of band theory was caused by its inadequate treatment of correlation effects. He realized that the correlations between the conduction electrons needed to be considered and that the one-electron approximation of band theory was not valid for a treatment of these effects.

In a series of papers[3,4,5] (for convenience we will refer to these as Hubbard I, II and III respectively) Hubbard has considered the

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simplest model for dealing with the problem of electron correlation in narrow band metals. The model is most often used in describing transition metals and their compounds (i.e. oxides and sulfides). The correlation effects appear in the form of an intra-site Coulomb repulsion between electrons. Hence what is essentially an infinite range force has been localized; that is the inter-site Coulomb force is completely screened. The Hubbard Hamiltonian in second-quantized notation is given by

$$H = \sum_{i,\sigma} \varepsilon_{i,\sigma} n_{i,\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} + t \sum_{\sigma} \sum_{\langle ij \rangle} (c_{i,\sigma}^{\dagger} c_{j,\sigma} + c_{j,\sigma}^{\dagger} c_{i,\sigma}) \quad (1.1)$$

where $\varepsilon_{i,\sigma}$ is the atomic energy gotten in some self-consistent manner, U is the intra-site Coulomb repulsion, and t is an overlap integral which is a measure of electron hopping between nearest neighbors (denoted on the summation by $\langle ij \rangle$). $c_{i,\sigma}$ ($c_{i,\sigma}^{\dagger}$) is the second-quantized operator which annihilates (creates) a Wannier electron on the site i with spin σ, and $n_{i,\sigma} = c_{i,\sigma}^{\dagger} c_{i,\sigma}$ counts the number of electrons.

In Hubbard I an equation-of-motion scheme for calculating the single-particle Green function was employed. Following the method of Zubarev[6] an approximate solution of the correlation problem is derived. The single-particle thermal Green function may be defined by

$$\langle\langle c_{i,\sigma}(t); c_{j,\sigma'}(0) \rangle\rangle = -i \, \Theta(t) \langle \{ c_{i,\sigma}(t), c_{j,\sigma'}^{\dagger}(0) \} \rangle \quad (1.2)$$

where $\Theta(t)$ is the unit step function, $\langle ... \rangle$ implies a thermal average, and $\{A,B\} = AB + BA$. Thus Green functions of this type obey the

following equation of motion

$$i\frac{d}{dt} << c_{i,\sigma}(t); \ c_{j,\sigma'}(0)>> = \delta(t)<\{c_{i,\sigma}(t), c_{j,\sigma'}^{\dagger}(0)\}>$$

$$+<<[c_{i,\sigma}(t),H]; \ c_{j,\sigma'}(0)>> \qquad (1.3)$$

It is often convenient to define the fourier transform

$$<< A;B>>_{\omega} = \int_{-\infty}^{\infty} << A(t); \ B(0)>> e^{i\omega t} \ dt \quad , \qquad (1.4)$$

where the energy $\omega(\hbar=1)$ is taken to be real. In this way all equations generated for the Green function will be algebraic. Hubbard then proceeded to investigate both the zero-bandwidth and finite-bandwidth problems. His solution to the finite-bandwidth problem has the property that it reduces to the exact atomic solution. Using the approximations proposed by Zubarav,

$$<< n_{i,\sigma} c_{k,\sigma}; \ c_{j,\sigma}^{\dagger}>>_{\omega} \cong < n_{i,-\sigma}> << c_{k,\sigma}; \ c_{j,\sigma}^{\dagger}>>_{\omega} \qquad (1.5a)$$

$$<< c_{i,-\sigma}^{\dagger} c_{k,-\sigma} c_{i,\sigma}; \ c_{j,\sigma}^{\dagger}>>_{\omega} \cong < c_{i,-\sigma}^{\dagger} c_{k,-\sigma}> << c_{i,\sigma}; c_{j,\sigma}>>_{\omega} \qquad (1.5b)$$

$$<< c_{k,-\sigma}^{\dagger} c_{i,-\sigma} c_{i,\sigma}; \ c_{j,\sigma}^{\dagger}>>_{\omega} \cong < c_{k,-\sigma}^{\dagger} c_{i,-\sigma}> << c_{i,\sigma}; \ c_{j,\sigma}^{\dagger}>>_{\omega} \qquad (1.5c)$$

Hubbard was able to de-couple the hierarchy of equations generated by the equation - of - motion method. He found that the pseudo-particle density of states split into two subbands for any finite value of the Coulomb term U. Each subband will contain exactly N states if one

chooses the unperturbed density of states to be symmetric about the center of the band. For the case where the ratio of the number of electrons to the number of sites is unity the lower subband will be completely full in the ground state and the system will be insulating. Hubbard realized the incorrectness of this result and in paper III he proposed a theory more consistent with the physical understanding of the problem. By introducing a critical value of the parameter U/Δ, where Δ = width of the single-electron energy band, he was able to show that splitting of the pseudo-particle density of states occurs only for those values of U/Δ greater than the critical value.

Another difficulty which was evident in paper I and which Hubbard corrected in paper III was that it predicted infinite pseudo-particle lifetimes. In paper I the basic assumption behind the Zubarev decoupling scheme was that the Green functions used described the motion of an electron say with spin ↑ as it was perturbed by the (assumed fixed) electrons with spin ↓. This system is then seen to be one where the electron motion is randomly modulated. In paper III, Hubbard modifies his theory to include the damping due both to disorder scattering and to the motions of the spin ↓ electrons. These corrections he refers to respectively as the scattering correction and the resonance broadening correction. Velicky et al.[7] showed Hubbard's scattering corrections to be identical to those obtained in the coherent potential approximation.[8]

Since the appearance of the pioneering work by Hubbard a great deal of literature has been devoted to systems described by the Hamiltonian given by equation (1). The model defined by this

Hamiltonian is used to study not only the metal-insulator transition, but also certain features of magnetic behavior in transition metals. The Hubbard model is essentially a two-parameter theory: the intra-site Coulomb repulsion U and the hopping energy t. Most work has been done for very large values of $|U/t|$ (localized moments)[9] and very small values of $|U/t|$ (itinerant model)[10]. Transition metals are probably best characterized by an intermediate value of $|U/t|$[11].

For the Hamiltonian given by equation (1.1) it has been proven that, for the half-filled band, the chemical potential is independent of the temperature[12]. As a result of this simplifying feature, most of the work on the Hubbard model has been devoted to the half-filled band. In particular, Lieb and Wu[13] have solved exactly the one-dimensional half-filled Hubbard model for zero temperature. They found the ground state to be anti-ferromagnetic with no Mott transition for finite values of the intrasite Coulomb energy U. The fact that very few exact results exist for the Hubbard model attests to the degree of difficulty of the problem. Hence any exact calculations are welcome regardless of the simplicity of the system.

In this study, we calculate the single-particle Green function exactly for the one-dimensional Hubbard dimer (2-sites) for arbitrary temperature and chemical potential. Other exact solutions to this problem also exist. Most recently Mei and Lee,[14] using a cluster variational approach, have solved the 2-site and 3-site eigenvalue problem for an extended Hubbard Hamiltonian exactly. They investigate the specific heat and magnetic susceptibility for arbitrary electron

density. Although not as comprehensive as the work of Mei and Lee

we believe that the work presented here has far greater calculational

potential in extensions to the linear chain and to higher dimensions.

We use the two-site Hubbard model as a testing ground for the

introduction of a new calculational method. The purpose of this study

is to develop the method on a model which has already been solved (in

part) and to compare with known results. The results which have the

greatest overlap with our present work were obtained by Ho and Barry,[15]

who looked at the half-filled dimer at high temperature, and with Chen

and Cheng[16] who looked at the thermodynamics of the extended Hubbard

dimer (inter-site electron interactions included) for arbitrary

electron density. Ho and Barry employed a cluster variation technique

which has its roots in the variational principle of statistical

mechanics. Essentially what is done is that a variational function $\bar{F}$

related to the free energy F of the N-particle system in equilibrium by

$$F = \min \bar{F} \qquad\qquad\qquad (1.6)$$

is considered to be a function of certain unknown correlation functions

of the system. Upon minimization with respect to these correlation

functions and the imposition of various normalization conditions, a

set of equations is generated for these correlation functions. Our

interest in this work derives from the fact that we too arrive at a

closed set of relations for the correlation functions of the system.

The work presented in this manuscript is more general in that we do not

put any restrictions either on the electron density or on the temperature. As a consequence of our being so general most of the results appearing here are new. The work of Chen and Cheng is also quite general and bears some discussion. Their approach was to solve the eigenvalue equation for the two-site extended Hubbard Hamiltonian

$$H = t \sum_{<ij>} \sum_{\sigma} c_{i,\sigma}^{\dagger} c_{j,\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} + V \sum_{<ij>} n_i n_j \qquad (1.7)$$

where t, U, $c_{i,\sigma}$, and $c_{i,\sigma}^{\dagger}$ and $n_{i,\sigma}$ are defined as before and the nearest-neighbor Coulomb term in V is included. Hence the range of the electron correlation is extended to include nearest neighbor interactions. Once the eigenvalues are known the partition function may be written down and the magnetic susceptibility can be calculated. While this procedure is rigorous for a finite number of sites, the calculation of the eigenvalues for a linear chain at present remains an impossible task.

We wish to emphasize that the one-dimensional Hubbard dimer does not simulate the real world, although it does seem to be an appropriate model for certain dimerized salts.[17-22] Our motivation for studying the Hubbard dimer is that it lends itself very well to the application of a new calculational method and that there exist other results for comparison.

The work in this study has been partitioned in the following manner. Chapter II is dedicated to laying down the basic foundations of the method. Here certain new concepts are introduced and related

to standard Green-function theory. Chapter III is an application of the method to the single-site Hubbard model. It is through this simple example that a number of skills are developed which prove to be of great importance in considering both the dimer and the linear chain. In chapter IV we study the Hubbard dimer in detail. It is in this example that the power of the method is fully manifested. The final chapter is a summary of our conclusions. We also cite our future expectations for using the method established in these pages.

II. METHOD

It is in this section that we focus our attention on the computational method for calculating the single-particle Green function. As is well known, Green functions are convenient tools in the study of interacting fields. Many properties of the system may be calculated once the Green functions are known. By system we are referring to a physical system describable by a given Hamiltonian formulated in second-quantized notation.

In practice the computation of Green functions for a non-trivial system must involve some sort of approximation scheme. At present there are three most standard methods of calculating Green functions: a decoupling scheme for their equations of motion, a diagrammatic perturbation expansion carried out in the interaction representation, and a moment expansion of the spectral weight function. As Bowen[23] has noted, contained in each of these approximation schemes are certain drawbacks.

The main criticism of the decoupling scheme as proposed by Zubarev[24] points to the ambiguity involved in the factorization of the higher-order correlation functions which appear in the Green-function equations of motion. The fact that a good approximation is obtained only if fluctuations of the factorized variables are very small is well known. Unfortunately, for factorizations of many higher-order correlation functions this requirement is known to fail.[25] To date there do not exist any appropriate higher-order factorizations which are

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sufficiently motivated by physical argument to be compelling.

In the diagrammatic method the theorem of Wick is used to evaluate the Green function by a perturbation expansion involving completely contracted field operators in the interaction representation. Using the fact that these contractions are just the free-field Green functions one may express the exact Green function in a series containing these free-field Green functions and also the interaction. This perturbative expansion may be expressed in a diagrammatic format so that various classes of diagrams can be grouped. This allows for many simplifications which would otherwise have been hidden by the complicated mathematical structure of the perturbation expansion. It is with regard to the very nature of this perturbation expansion that criticism arises. The validity and convergence properties of expanding the exact Green function in terms of the non-interacting Green function becomes questionable in highly correlated systems. Also, by expanding in powers of the interaction convergence of the series is not guaranteed and methods of renormalization are needed. Another difficulty in dealing with the diagrammatic perturbation expansion is that, if one tries to account for correlation effects by including electronic correlation terms as part of the unperturbed Hamiltonian, Wick's theorem no longer holds[26], because the perturbation expansion for the Green function (Matsubara[27]) then contains commutators which are no longer c-numbers. Approximation schemes for this problem have been worked out by Robert et al. and more recently by Anda[28] for hybridised electronic bands. Each of these schemes contains some sort of mean-field type of approximation.

The third method of calculation of the Green function was proposed by Lonke[29,30]. This method investigates the first 2N moments of the single particle spectral weight function and is based on the mathematical theory of the classical moment problem. The Nth moment of the spectral weight function can be shown to be related to the Nth operation of the Liouville operator, L, defined by

$$L\theta = [\theta, H]$$
(2.1)

for any operator θ where H is the Hamiltonian of the system. Calculation of the entire spectrum of moments is an impossible task. This means that the dynamical properties as well as the statistical mechanics of the system must be calculated from an incomplete set of quantities, namely a finite number of moments of the spectral weight function. Problems also arise in finding a consistent approximation when one looks at the thermodynamic limit.

The method we use in this manuscript has its roots in the moment technique of Lonke. The Fourier transform of the single-particle fermion Green function may be expressed as a moment expansion. This can be seen by looking at the Heisenberg equation of motion for this single-particle Green function:

$$i \frac{dG}{dt} = i \frac{d}{dt} <<c(t); c^\dagger(0)>> = \delta(t) <\{c(t), c^\dagger(0)\}> + << [c,H]; c^\dagger>>.$$
(2.2)

We may express the last term on the right hand side in terms of the Liouville operator via

$$LA = [A,H]$$
(2.3)

Upon taking the Fourier transform of both sides of (2.2) we arrive at

$$\omega << c;c^{\dagger} >>_{\omega} = <\{c,c^{\dagger}\}> + << Lc;c^{\dagger} >>_{\omega} \quad . \tag{2.4}$$

By making the replacement $c \rightarrow Lc$ in equation (2.4) and noting that

$$L^2 c = [[c,H],H] \quad , \tag{2.5}$$

we have

$$\omega << Lc;c^{\dagger} >>_{\omega} = <\{Lc,c^{\dagger}\}> + << L^2 c;c^{\dagger} >>_{\omega} \quad . \tag{2.6}$$

Now placing equation (2.6) into the right hand side of equation (2.4) we see that

$$<< c;c^{\dagger} >>_{\omega} = \frac{1}{\omega} <\{c,c^{\dagger}\}> + \frac{1}{\omega^2} <\{Lc,c^{\dagger}\}>$$

$$\tag{2.7}$$

$$+ \frac{1}{\omega^2} << L^2 c;c^{\dagger} >>_{\omega} \quad .$$

We may repeat the procedure by replacing c with Lc in equation (2.7), thus producing a term proportional to $L^3 c$. It is then seen that a moment expansion is being generated:

$$G(\omega) = << c;c^{\dagger} >>_{\omega} = \sum_{n=0}^{\infty} \frac{1}{\omega^{n+1}} <\{L^n c,c^{\dagger}\}> \quad . \tag{2.8}$$

We next introduce the concept of a normalizable manifold of linear operators. This manifold is a Hilbert space with a basis chosen to be second-quantized operators of a particular ("fermion") type. Crawford[31] was the first to deal with this operator space, which he chose to call the associated Hilbert space. The elements of this space are linear

combinations of products of an odd numbers of fermion creation and/or annihilation operators. Crawford attempted to use this operator space as a means of quantizing fields in an alternate manner. It is our aim to exploit the properties of this space for different purposes. We call this Hilbert space of linear second-quantized operators a (fermion) superspace, and we refer to operators on superspace elements (or vectors) as superoperators[32]. These superoperators play the same role as operators (matrices) do in ordinary Hilbert space. As a first example we note that the Liouville operator L is a superoperator in our super-space; it can be shown to be hermitian in this superspace if H is hermitian and commutes with the density operator[33]. In mathematical language the operation of these superoperators on superspace vectors effect the mapping of operators on operators. As a reminder we mention the mappings with which physicists are most familiar: the mappings of objects on objects which are referred to as operators, the mappings of objects on numbers which are called functionals, and mappings of numbers on numbers called functions. As in the formulation of standard second-quantized field theory only those superoperators which preserve the linearity of the superspace will play a fundamental role in our theory.

At this point we wish to stress the fact that, although our super-space is completely analogous to the "ordinary" Hilbert space of quantum mechanics, there exist a couple of novel features which we now delineate. The first concerns the definition of a scalar product of two (fermion) superspace vectors A and B. This is defined to be the thermal average,

taken in the grand canonical ensemble, of the anti-commutator of the two "vectors" (linear operators):

$$((A,B)) = <\{B, A^\dagger\}> \ .$$ (2.9)

It can be seen then that the norm of a vector in the superspace will usually contain thermal averages and therefore depend on temperature and chemical potential.

For a given orthonormal basis in Hilbert space, it is possible to equate matrix elements of the resolvent operator taken with respect to this basis, to a formal moment expansion as follows:

$$<k|(\omega-H)^{-1}|k'> = \sum_{n=0}^{\infty} \frac{1}{\omega^{n+1}} <k|(H)^n|k'> \ .$$ (2.10)

This is a consequence of the binomial theorem

$$(1+x)^m = \sum_{p=0}^{\infty} \frac{m(m-1)\ldots(m-p+1)}{p!}$$ (2.11)

where it is required that $|x|<1$. As can be seen from equations (2.8), (2.9) and (2.10) the Fourier time-transform of the single-particle Green function may be written as a superspace matrix element of the resolvent of the Liouville operator[34]:

$$G(\omega) = << c;c^\dagger >>_\omega = ((c, (\omega-L)^{-1} c)) \ .$$ (2.12)

We propose to study the single-particle Green function in this form. We note that the problem of evaluation of the Green function has been re-cast into a matrix inversion problem in superspace.

The reason for calculating the Green function in this manner is motivated by a theorem by Masson[35]. This theorem states that for any Hamiltonian operator, bounded or unbounded, the matrix elements of its N-dimensional resolvents converge, as $N \to \infty$, to the matrix elements of the exact resolvent for any complex value of ω which is not contained in the spectrum of the Hamiltonian. Unlike the case for perturbation expansions, this theorem guarantees convergence regardless of the nature of the interactions, i.e. for any Hamiltonian.

We now consider the evaluation of the single-particle Green function,

$$G(\omega) = ((c, (\omega - L)^{-1} c)) , \qquad (2.13)$$

where the matrix element refers to the superspace. Evaluation of this matrix element involves finding the eigenvalues of the Liouville operator L:

$$L\psi_i = [\psi_i, H] = \lambda_i \psi_i ,$$

where the operators ψ_i are linear combinations of operators ϕ_α which are products of an odd number of fermion operators like c and $c^\dagger$. Assuming this to be done, at least for finite systems, we can expand the single-particle operator c by

$$c = \sum_i b_i \psi_i , \qquad (2.14)$$

where the c-number coefficients b_i contain certain thermal averages which arise from normalization of the ψ_i's in the superspace. Judd[36]

introduced a clever representation for fermion superspace elements like the operators ϕ_α, which he called shift operators. It is in this representation, to be discussed later, that our method derives its strength and henceforth we refer to such operators as Judd operators. Judd noted that these operators ϕ_α are elements of a semi-simple Lie algebra[37]. A property of these semi-simple Lie algebras is that they regenerate themselves under commutation operations. These commutation relations are most easily expressed in terms of a Euclidean space R_ℓ which contains a positive metric. The complete group theoretical nature of this Lie algebra necessarily leads one into discussions of root vectors and root spaces[38]. Those root vectors which are independent may be shown to span the Euclidean space R_ℓ. An iso-morphism exists between semi-simple algebras of rank ℓ and sets of roots in an ℓ-dimensional space R_ℓ. This isomorphism is accomplished by means of the canonical commutation relations

$$[h_i, h_j] = 0 \tag{2.15a}$$

$$[\vec{h}, \phi_\alpha] = \vec{\alpha}\,\phi_\alpha \tag{2.15b}$$

$$[\phi_\alpha, \phi_\alpha^\dagger] = \vec{\alpha} \cdot \vec{h} \tag{2.15c}$$

$$[\phi_\alpha, \phi_\beta] = N_{\alpha,\beta}\,\phi_{\alpha+\beta} \tag{2.15d}$$

where ϕ_α are the Judd operators, $\vec{\alpha}$ are the root vectors, the h_i are orthogonal projection operators which constitute a Cartan sub-algebra and $N_{\alpha,\beta}$ are the remaining non-zero structure constants for the group.

It is in the expansion of the single-particle operators c in terms of the Judd operators that our method takes its initiative. We now examine the explicit structure of these operators. In the context of a given atomic shell, one may express a given state $|\psi\rangle$ in Fock space as a product of second-quantized creation operators in some given canonical ordering, acting on a well defined "vacuum" state $|0\rangle$;

$$|\psi\rangle = A_N^\dagger \, |0\rangle = c_1^\dagger \, c_2^\dagger \cdots \, c_N^\dagger \, |0\rangle \qquad (2.16)$$

This defines the operator $A_N^\dagger$. The subscripts here refer to different electron states in a given shell. Thus in a filled s-shell N=2, in a filled p-shell N=6, in a filled d-shell N=10, and so forth. Similarly we may define the operator A_N as follows:

$$A_N = c_N \, c_{N-1} \cdots \, c_2 \, c_1 \qquad (2.17)$$

where we note the sequence of second-quantized destruction operators is taken in reversed canonical order. We now construct the Judd operator

$$\phi = A_N^\dagger \, I_\theta \, A_M' \quad , \qquad (2.18)$$

where the idempotent operator I_θ is known as the invariant of the shell and is given by

$$I_\theta = A_\theta \, A_\theta^\dagger \quad . \qquad (2.19)$$

The operators A_θ and $A_\theta^\dagger$ are, respectively, products of annihilation and creation operators in the canonical ordering for the filled shell. The

operator I_θ is a projection operator for the "vacuum" in ordinary

Fock space. The advantages of expressing the Judd operators in

this manner are manifested in the simplicity obtained when calculating

scalar products in superspace and also because it automatically gives

the canonical commutation relations for the Lie algebra. By looking

at the structure of the operators ϕ as we have constructed them in

equation (2.18), we can see that they have the form of a stepping (or

shift) operator if $M \neq N$. This stepping operator destroys a given

configuration A_M^t in the shell, then proceeds to create a new configura-

tion $A_N^\dagger$. In the context of condensed-matter physics one would say that

these Judd operators are many-particle stepping operators which allow

one to step between many-particle states differing by M-N electrons.

The structure of these Judd stepping operators is such that they may be

characterized as having a net spin S. We define the net spin to be the

spin difference between initial and final configurations:

$$S = S_M - S_N \tag{2.20}$$

The greater the spin degeneracy for the M-electron and N-electron

configurations, the larger the number of possible transitions differing

by N-M electrons. Hence we can see that the inclusion of spin greatly

increases the number of Judd operators to be considered.

We use the Judd stepping-operator formalism to calculate the

single-particle Green function for the two-site Hubbard model. By ex-

panding the single-particle operators c in terms of the Judd operators

which are eigenfunctions of the Liouville operator, we are able to

solve for the single-particle Green function of the Hubbard dimer

exactly. By working with the Judd operators we are explicitly solving exactly a simple many-body problem. From the very structure of these operators we see that one can easily surpass any type of mean-field approximation. The fact that the equations of motion for these stepping operators is investigated necessarily requires that the detailed structure of the "shell" becomes important. A point that needs to be stressed is that all possible configuration fluctuations of the "shell" are contained in the set of Judd operators. It is the primary purpose of this study to determine those operators, for both the single-site Hubbard model and the Hubbard dimer, which are physically the most relevant. In this way it is planned that some type of systematic approximation to the linear chain may be obtained.

Recall the expression for the Fourier transform of the single-particle Green function:

$$G(\omega) = ((c, (\omega-L)^{-1} c)) \quad , \tag{2.21}$$

where the matrix element of the resolvent operator refers to the super-space. The calculation proceeds by expressing the single-particle operator c in terms of the eigenstates ψ_i of the Liouville operator:

$$c = \sum_i b_i \, \psi_i \, , \tag{2.22}$$

where

$$L \, \psi_i = \lambda_i \, \psi_i \quad . \tag{2.23}$$

The eigenstates are in turn expressed as linear combinations of Judd operators ϕ which step between Fock-space states with N and N-1 fermions. It is through these Judd operators, which recall are stepping operators between many-particle states, that properties of the correlated system are manifested. By solving the eigenvalue problem for the Liouville operator, L, we are simultaneously diagonalizing its resolvent matrix. The difficulty of this task is reduced appreciably when one takes advantage of both the symmetries of the Hamiltonian and (to a lesser extent) the Lie group structure of the Judd operators. Having solved the eigenvalue equation one may express the single-particle Green function by

$$G(\omega) = \sum_i \frac{|b_i|^2}{\omega - \lambda_i} \ ((\psi_i, \psi_i)) \ , \tag{2.24}$$

where the eigenfunctions are of course orthogonal:

$$((\psi_i, \psi_j)) = 0 \ , \quad i \neq j \ . \tag{2.25}$$

From the definition of a scalar product on the superspace we see that the Green function is expressed as a sum of thermal averages of various correlation functions.

We then make use of the dispersion relation

$$<\psi_i^\dagger \ \psi_i> = \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \ f_o(\omega) \ \text{Im} \ ((\psi_i, \ (\omega - i\delta - L)^{-1} \ \psi_i)) \ , \tag{2.26}$$

where $f_o(\omega)$ is the fermi function defined by

$$f_o(\omega) = (1 + e^{\beta(\omega-\mu)})^{-1} \qquad (2.27)$$

and $\beta = (kT)^{-1}$ with T = absolute temperature, μ = chemical potential and k being Boltzmann's constant. Equation (2.26) simplifies to

$$<\psi_i^\dagger \psi_i> = f_o(\lambda_i) \ ((\psi_i, \psi_i)) \qquad (2.28)$$

for

$$L\psi_i = \lambda_i \psi_i \ . \qquad (2.29)$$

By using the set of coupled linear inhomogeneous equations given by equation (2.28) one can solve for the individual correlation functions in terms of the fermi functions $f_o(\lambda_i)$. In practice, the algebraic decoupling is somewhat tedious and the computer is used to study the thermal properties.

We see then that the Green function may be calculated exactly for selected systems, using this technique. The advantages are in the systematics of the method, and in the fact that the treatment of highly correlated systems appears to be natural. It is the purpose of this study to illustrate the method by applying it to both the single-site Hubbard model and to the Hubbard dimer. Exact results are obtained and comparisons are made with previous exact results and with various approximation schemes.

III. SINGLE SITE

We now carry out the task of solving a relatively trivial example in order to illustrate the various new concepts introduced in the previous chapter. We analyze the single-site s-band Hubbard model with the obvious intention of gaining insight into the more difficult problem of the Hubbard dimer. Also, any solution for the dimer must reduce, in the atomic limit, to the single-site solution.

As a first step, we wish to write the invariant, I_θ, for the single-site s-shell. To do this we choose the canonical ordering for the annihilation operators to be $c_\downarrow c_\uparrow$ where the subscripts refer to spin-down and spin-up electrons, respectively. Then the invariant I_θ is

$$I_\theta = c_\downarrow c_\uparrow c_\uparrow^\dagger c_\downarrow^\dagger = (1-n_\uparrow)(1-n_\downarrow) \quad .$$

Once the invariant is written down we need to establish the set of Judd operators which are relevant. We are interested in calculating the single-particle Green function which is written with respect to the single-particle annihilation operator $c_\uparrow$:

$$G_\uparrow(\omega) = ((c_\uparrow (\omega-L)^{-1} c_\uparrow)) \quad . \tag{3.1}$$

The single particle annihilation operator $c_\uparrow$ is in turn expanded in terms of single-particle Judd operators only. Hence only those Judd stepping operators having the form

$$\phi = A_{n-1}^\dagger I_\theta A_n' \tag{3.2}$$

will contribute to the spectrum of the single-particle Green function.

Note that the Lie algebra structure also allows Judd operators of the form

$$\phi = A^{\dagger}_{n,s} \, I_{\theta} \, A'_{n+1,s\pm3/2} \quad , \tag{3.3}$$

i.e. the particle number changes by one while the net spin changes by more than 1/2. The fact that the Hubbard Hamiltonian does not involve interactions which flip spin permits one to ignore operators of this type. The physics of this reasoning manifests itself in the expansion of the single-particle creation and annihilation operators in terms of Judd operators of the form given in equation (3.2).

The Hamiltonian for the single-site s-band Hubbard model is given in second-quantized notation by

$$H = \epsilon(n_{\uparrow} + n_{\downarrow}) + U \, n_{\uparrow} \, n_{\downarrow} \quad , \tag{3.4}$$

where $n_{\uparrow} = c^{\dagger}_{\uparrow} c_{\uparrow}$, etc. We see then that the single site can accommodate four states:

Number of electrons	Spin	Energy
0	0	0
1	$\uparrow$	ϵ
1	$\downarrow$	ϵ
2	$\uparrow\downarrow$	$2\epsilon+U$

where U is the (repulsive) Coulomb interation. The Judd operators that we need to consider then are those which represent transitions from the two-electron state to one of the single-electron states, and from one of the single-electron states to the state of no electrons. For

the purpose of illustration we will work through the complete U(4) Lie

algebra for the single site.

Recall the canonical commutation relations for semi-simple Lie

algebras:

$$[h_i, E_\alpha] = \alpha_i E_\alpha \qquad (3.5a)$$

$$[h_i, h_j] = 0 \qquad (3.5b)$$

$$[E_a, E_\alpha^\dagger] = \vec{\alpha} \cdot \vec{h} \qquad (3.5c)$$

$$[E_\alpha, E_\beta] = N_{\alpha,\beta} E_{\alpha+\beta} \qquad (3.5d)$$

where the h_i are the orthogonal projection operators, the E_α are the

stepping operators associated with the root vector $\vec{\alpha}$ and the $N_{\alpha,\beta}$ are

the structure constants of the group. Following Bowen[39] we may write

the one-particle stepping operators for the single-site:

$$E_\alpha = \phi_\uparrow^{(-)} = I_\theta c_\uparrow \qquad (3.6a)$$

$$E_{\alpha'} = \phi_\downarrow^{(-)} = I_\theta c_\downarrow \qquad (3.6b)$$

$$E_\beta = \phi_\uparrow^{(+)} = c_\uparrow^\dagger I_\theta A_\theta \qquad (3.6c)$$

$$E_\beta = \phi_\uparrow^{(+)} = c_\downarrow^\dagger I_\theta A_\theta \qquad (3.6c)$$

where $A_\theta = c_\downarrow c_\uparrow$. The two particle stepping operator is given by

$$E_\gamma = \phi_2 = I_\theta A_\theta \qquad (3.7)$$

and the spin-flip operator which leaves the number of particles unchanged

is

$$E_\delta = \phi_3 = c_\uparrow^\dagger \, I_\theta \, c_\downarrow \quad . \tag{3.8}$$

We now need to write down the orthogonal projection operators, h_i, which comprise the Cartan sub-algebra. Note that the structure of these projection operators is such that the single-particle operators appearing to the left of the invariant I_θ are just the hermitian conjugates of those operators appearing on the right of the invariant;

$$h_o = I_\theta = c_\downarrow \, c_\uparrow \, c_\uparrow^\dagger \, c_\downarrow^\dagger = A_\theta \, A_\theta^\dagger \tag{3.9a}$$

$$h_1 = c_\uparrow^\dagger \, I_\theta \, c_\uparrow \tag{3.9b}$$

$$h_2 = c_\downarrow^\dagger \, I_\theta \, c_\downarrow \tag{3.9c}$$

$$h_3 = c_\uparrow^\dagger \, c_\downarrow^\dagger \, I_\theta \, c_\downarrow \, c_\uparrow = A_\theta^\dagger \, I_\theta \, A_\theta \quad . \tag{3.9d}$$

We now make the following observation. We see that, for the single-site s-band Hubbard model, choosing the appropriate stepping operators and orthogonal projection operators was a relatively simple matter. The reason for this was that our choice was motivated by the physics of our system, which, in this case, was very transparent. However, for non-trivial systems, such as mixed-valence compounds, choosing the physically important operators requires further insight. This point will be discussed in greater detail in the last chapter of this study.

Once the stepping operators and the projection operators are known, one may calculate the root vectors from

$$[h_i, E_\alpha] = \alpha_i \, E_\alpha \tag{3.10a}$$

$$[h_i, E_{\alpha'}] = \alpha_i' E_{\alpha'} \tag{3.10b}$$

where α_i, α_i' are the four-tuples

$$\vec{\alpha} = (\alpha_o, \alpha_1, \alpha_2, \alpha_3) \tag{3.11a}$$

$$\vec{\alpha}' = (\alpha_o', \alpha_1', \alpha_2', \alpha_3') \quad . \tag{3.11b}$$

As an illustration we calculate the root vector $\vec{\alpha}$ explicitly:

$$[h_o, E_\alpha] = (+1) E_\alpha = \alpha_o E_\alpha \tag{3.12a}$$

$$[h_1, E_\alpha] = (-1) E_\alpha = \alpha_1 E_\alpha \tag{3.12b}$$

$$[h_2, E_\alpha] = (0) E_\alpha = \alpha_2 E_\alpha \tag{3.12c}$$

$$[h_3, E_\alpha] = (0) E_\alpha = \alpha_3 E_\alpha \quad . \tag{3.12d}$$

Similarly we find

$$\vec{\alpha}' = (1, 0, -1, 0) \tag{3.14}$$

$$\vec{\beta}' = (0, 1, 0, -1) \tag{3.15}$$

$$\vec{\beta}' = (0, 0, 1, -1) \tag{3.16}$$

$$\vec{\gamma} = (1, 0, 0, -1) \tag{3.17}$$

$$\vec{\delta} = (0, 1, -1, 0) \tag{3.18}$$

Having written down the Lie algebra structure of the single-site we now proceed to calculate the single-particle Green function

$$G_\sigma(\omega) = ((c_\sigma(\omega-L)^{-1} c_\sigma)) \quad , \tag{3.19}$$

where $\sigma = \uparrow, \downarrow$.

The single-particle annihilation operators $c_\uparrow$, $c_\downarrow$, can be expanded in terms of the stepping operators:

$$c_\uparrow = \phi_\uparrow^{(-)} + \phi_\uparrow^{(+)} = E_\alpha + E_\beta, \tag{3.20a}$$

$$c_\downarrow = \phi_\downarrow^{(-)} + \phi_\downarrow^{(+)} = E_{\alpha'} + E_\beta \quad . \tag{3.20b}$$

We will look at $G_\uparrow(\omega)$ only, hence expansion (3.20a) will be used. From the definition of E_α and E_β, we may write

$$E_\alpha = I_\theta c_\uparrow = (1-n_\uparrow)(1-n_\downarrow)c_\uparrow = (1-n_\downarrow)c_\uparrow \tag{3.21a}$$

$$E_{\beta'} = c_\downarrow^\dagger I_\theta c_\downarrow c_\uparrow = c_\downarrow^\dagger(1-n_\uparrow)(1-n_\downarrow)c_\downarrow c_\uparrow = n_\downarrow c_\uparrow , \tag{3.21b}$$

where we have used

$$n_\sigma c_\sigma = 0 \quad , \quad n_\sigma c_\sigma^\dagger = c_\sigma^\dagger \tag{3.22a}$$

$$c_\sigma n_\sigma = c_\sigma \quad , \quad c_\sigma^\dagger n_\sigma = 0 \quad . \tag{3.22b}$$

Normalizing E_σ and $E_{\sigma'}$ we have, respectively,

$$\phi_\uparrow^{(-)} = \frac{(1-n_\downarrow)}{(1-\langle n_\downarrow \rangle)^{\frac{1}{2}}} c_\uparrow \tag{3.23a}$$

$$\phi_\uparrow^{(+)} = \frac{n_\downarrow}{\langle n_\downarrow \rangle^{\frac{1}{2}}} c_\uparrow \quad . \tag{3.23b}$$

Now operating with the Liouville operator gives

$$L \ \Phi_\uparrow^{(\pm)} = [\ \Phi_\uparrow^{(\pm)}, \ H\ ] = \epsilon^{(\pm)} \ \Phi_\uparrow^{(\pm)} \ , \tag{3.24}$$

where $\epsilon^{(\pm)} = \epsilon + \frac{1}{2} U \pm \frac{1}{2} U$. Recall that the Judd operators $\Phi_\uparrow^{(\pm)}$ are an orthonormal basis of eigenfunctions of the Liouville operator which contain a product of an odd number of fermion single-particle operators. We may now write the single-particle Green function as[40]

$$G_\uparrow(\omega) = \sum_r \frac{<N_\downarrow^{(r)}>}{\omega - \epsilon^{(r)}} \ , \tag{3.25}$$

where $r = \pm 1$ and $N_\downarrow^{(r)}$ is equal to $n_\downarrow$ for $r = +1$ and $(1-n_\downarrow)$ for $r = -1$. In this notation, the one-electron operator may be expressed as

$$c_\uparrow = \sum_r <N_\downarrow^{(r)}>^{\frac{1}{2}} \Phi_\uparrow^{(r)} \ . \tag{3.26}$$

It is a straightforward matter to calculate the thermal average $<n_\uparrow> = <c_\uparrow^\dagger c_\uparrow>$ using the dispersion relation

$$<A^\dagger B> = \int_{-\infty}^{\infty} \frac{d\omega}{\pi} f_o(\omega) \ \mathrm{Im} \ ((B, \ (\omega - i\delta - L)^{-1} A)) \ , \tag{3.27}$$

which simplifies to

$$<A^\dagger B> = ((B, \ A)) \ f_o(E_a) \tag{3.28}$$

for $LA = E_a A$ with $f_o(E_a) = (e^{\beta(E_a - \mu)} + 1)^{-1}$.

We have

$$<c_\uparrow^\dagger c_\uparrow> = <n_\uparrow> = (1 - <n_\downarrow>) f^{(-)} + <n_\downarrow> \ f^{(+)} \ , \tag{3.29}$$

where

$$f^{(\pm)} = (e^{\beta(\epsilon-\mu)} + 1)^{-1} = \langle \phi^{(\pm)\dagger} \phi^{(\pm)} \rangle \quad . \tag{3.30}$$

In the absence of a magnetic field $\langle n_\uparrow \rangle = \langle n_\downarrow \rangle = \langle n \rangle$ and we may solve (3.29) for $\langle n \rangle$:

$$\langle n \rangle = (1 - \langle n \rangle) f^{(-)} + \langle n \rangle f^{(+)} \quad \text{or}$$

$$\langle n \rangle = \frac{f^{(-)}}{1 + f^{(-)} - f^{(+)}} \quad . \tag{3.31}$$

In order to solve for the correlation function $\langle n_\uparrow n_\downarrow \rangle$ we look at $\langle c_\uparrow^\dagger \phi_\uparrow^{(+)} \rangle$ and use equation (3.28). We arrive at

$$\langle \phi_\uparrow^{(+)\dagger} c_\uparrow \rangle = \frac{\langle n_\uparrow n_\downarrow \rangle}{\langle n_\uparrow \rangle^{\frac{1}{2}}} = ((c_\uparrow, \phi_\uparrow^{(+)})) f^{(+)} \quad \text{or} \tag{3.32a}$$

$$\frac{\langle n_\uparrow n_\downarrow \rangle}{\langle n_\downarrow \rangle^{\frac{1}{2}}} = \langle n_\uparrow \rangle^{\frac{1}{2}} f^{(+)} \quad . \tag{3.32b}$$

Once again, since we assume no magnetic field, $\langle n_\uparrow \rangle = \langle n_\downarrow \rangle = \langle n \rangle$, then equation (3.32b) simplifies to

$$\langle n_\uparrow n_\downarrow \rangle = \langle n \rangle f^{(+)} \quad . \tag{3.33}$$

From equation (3.31) this becomes

$$\langle n_\uparrow n_\downarrow \rangle = \frac{f^{(-)} f^{(+)}}{1 + f^{(-)} - f^{(+)}} \quad . \tag{3.34}$$

We therefore have an exact result for the single-site which agrees with that of Hubbard I.

IV. HUBBARD DIMER

It is the purpose of this chapter to solve the Hubbard dimer problem exactly using the Judd operator formalism. First we will summarize our approach and reiterate our method.

The Fourier transform of the single-particle Green function may be written as a matrix element of the resolvent operator $(\omega-L)^{-1}$, where L is the Liouville operator:

$$G(\omega) = ((c, (\omega-L)^{-1} c)) \quad .$$

This matrix element is defined in a Hilbert space (called superspace) where elements are products of odd numbers of second-quantized fermion operators. In this format we may express the single-particle operators c in terms of orthogonal basis elements ψ of the superspace:

$$c = \sum_i b_i \psi_i \quad . \tag{4.1}$$

In this work the ψ_i are taken to be eigenvectors of the Liouville operator and are linear combinations of operators ϕ which are products of an odd number of fermion operators such as c and $c^\dagger$.

In order to evaluate the resolvent matrix elements for the Hubbard (s-band) dimer we must first solve the eigenvalue equation for the Liouville operator using the Hamiltonian

$$H = \sum_{i,\sigma} \varepsilon_i \, n_{i,\sigma} + U\sum_i n_{i,\sigma} \, n_{i,-\sigma} + t \sum_\sigma (c^\dagger_{1,\sigma} \, c_{2,\sigma} + c^\dagger_{2,\sigma} \, c_{1,\sigma}),$$
$$\tag{4.2}$$
$$i = 1,2 \quad \sigma = \uparrow,\downarrow \quad .$$

This task is facilitated by exploiting certain symmetries of the Hamiltonian. As will be seen, these symmetries include site-exchange invariance and spin-flip invariance. We construct eigenvectors ψ of the Liouville operator which are expressed in terms of the ϕ operators in a manner which takes full advantage of the symmetries of the Hamiltonian. Recall that the ϕ operators in question are single-particle stepping operators in the superspace. That is to say they step from many-particle states having N+1 electrons with net spin S, to many-particle states containing N particles with net spin $S\pm\frac{1}{2}$. We then expand the single-particle annihilation operator c in terms of the ψ 's and proceed to calculate the single-particle Green function. The Green function is therefore expressed as a linear combination of thermal averages of correlation functions. Recall that these thermal averages arise naturally in the definition of scalar product and vector norm in the superspace. These thermal averages are, in turn, determined by the dispersion relation

$$<A^\dagger B> = \int_{-\infty}^{\infty} \frac{d\omega}{\pi} f(\omega) \, Im \, ((B, (\omega-i\delta-L)^{-1} A)) \; . \tag{4.3}$$

Upon diagonalization of the Liouville operator in the space of appropriate single-particle stepping operators:

$$L\psi_i = [\psi_i, H] = \lambda_i \psi_i \; , \tag{4.4}$$

the dispersion relation relations for the $<\psi_i^\dagger \psi_i>$ simplify to take the form

$$<\psi_i^\dagger \psi_i> = ((\psi_i, \psi_i)) \, f_o(\lambda_i) \; . \tag{4.5}$$

We must therefore solve a set of inhomogeneous linear equations typically in the form of equations (4.5) for the correlation functions. Once these correlation functions are known the Green function is also known and hence thermodynamic quantities may be calculated. Now that we have sketched our format, we proceed to solve the Hubbard s-band dimer problem (the Hubbard model for two sites) exactly.

As was stated previously the first step in solving a problem in this formalism is to write down a canonical ordering of operators and stick to it. We do this by writing the invariant for the s-band Hubbard dimer as

$$I_\theta = c_{2\downarrow} \, c_{2\uparrow} \, c_{1\downarrow} \, c_{1\uparrow} \, c_{1\uparrow}^\dagger \, c_{1\downarrow}^\dagger \, c_{2\uparrow}^\dagger \, c_{2\downarrow}^\dagger$$

$$\tag{4.6}$$

$$= (1-n_{1\uparrow})(1-n_{1\downarrow})(1-n_{2\uparrow})(1-n_{2\downarrow}) \quad .$$

Once the canonical ordering has been chosen, we may write down the expansion of the single-particle operator $c_{1\uparrow}$ in terms of the Judd operators ϕ_i given by

$$\phi_i = A_i^\dagger \, I_\theta \, A_i' \quad . \tag{4.7}$$

To obtain this expansion we are guided by the analogy of the single site. For the dimer we simply sum the atom-like operators for each site. Thus the expansion will contain eight Judd operators,

$$c_{1\uparrow} = \phi_1 + \phi_2 + \phi_3 + \phi_4 + \phi_5 + \phi_6 + \phi_7 + \phi_8 \quad , \tag{4.8}$$

where the Judd operators ϕ_i are given by

$$\phi_1 = I_\theta \, c_{1\uparrow} = (1-n_{1\downarrow})(1-n_{2\uparrow})(1-n_{2\downarrow}) \, c_{1\uparrow}$$

$$\phi_2 = c_{1\downarrow}^\dagger \, I_\theta \, c_{1\downarrow} \, c_{1\uparrow} = (1-n_{2\uparrow})(1-n_{2\downarrow}) \, n_{1\downarrow} \, c_{1\uparrow}$$

$$\phi_3 = c_{2\uparrow}^\dagger \, I_\theta \, c_{2\uparrow} \, c_{1\uparrow} = (1-n_{1\downarrow})(1-n_{2\downarrow}) \, n_{2\uparrow} \, c_{1\uparrow}$$

$$\phi_4 = c_{2\downarrow}^\dagger \, I_\theta \, c_{2\downarrow} \, c_{1\uparrow} = (1-n_{1\downarrow})(1-n_{2\uparrow}) \, n_{2\downarrow} \, c_{1\uparrow}$$

$$\phi_5 = c_{1\downarrow}^\dagger \, c_{2\uparrow}^\dagger \, I_\theta \, c_{2\uparrow} \, c_{1\downarrow} \, c_{1\uparrow} = (1-n_{2\downarrow}) \, n_{2\uparrow} \, n_{1\downarrow} \, c_{1\uparrow}$$

$$\phi_6 = c_{1\downarrow}^\dagger \, c_{2\downarrow}^\dagger \, I_\theta \, c_{2\downarrow} \, c_{1\downarrow} \, c_{1\uparrow} = (1-n_{2\uparrow}) \, n_{2\downarrow} \, n_{1\downarrow} \, c_{\uparrow}$$

$$\phi_7 = c_{2\uparrow}^\dagger \, c_{2\downarrow}^\dagger \, I_\theta \, c_{2\downarrow} \, c_{2\uparrow} \, c_{1\uparrow} = (1-n_{1\downarrow}) \, n_{2\downarrow} \, n_{2\uparrow} \, c_{1\uparrow}$$

$$\phi_8 = c_{1\downarrow}^\dagger \, c_{2\uparrow}^\dagger \, c_{2\downarrow}^\dagger \, I_\theta \, c_{2\downarrow} \, c_{2\uparrow} \, c_{1\downarrow} \, c_{1\uparrow} = n_{2\downarrow} \, n_{2\uparrow} \, n_{1\downarrow} \, c_{1\uparrow}$$

It is important to note the structure of these operators: ϕ_1 is a stepping operator from a state having one particle to the empty state, ϕ_2, ϕ_3 and ϕ_4 are stepping operators from states having two particles to single-particle states, ϕ_5, ϕ_6 and ϕ_7 are the stepping operators from states having three particles to two-particle states, and ϕ_8 is a stepping operator from the state having four particles to a three-particle state. We see that the ϕ operators involved in the expansion of the single-particle operator $c_{1\uparrow}$ are also single-particle operators. By this we mean that the set of ϕ's step between states having N+1 particles and states having N particles. This group of single-particle stepping operators constitutes a subset of the Lie algebra for the group U(16). (The complete Lie algebra contains two-particle stepping operators involving transitions of the type 2→0, 3→1 and 4→2; three-

particle stepping operators involving transitions of the type $3\rightarrow 0$, $4\rightarrow 1$; and the four particle stepping operators involving the transition of the type $4\rightarrow 0$. The complete Lie algebra structure for the Hubbard s-band dimer is given in appendix (A).) It is the purpose here to focus our attention only on those single-particle operators which are relevant to the calculation of the single-particle Green function.

At this point it becomes necessary to introduce the site-exchange operator P. This operator has the following properties:

$$P^2 = 1 \ , \ P^{-1} = P, \ Pc_{1,\sigma} \ P^{-1} = c_{2,\sigma}, \ Pc_{2,\sigma} \ P^{-1} = c_{1,\sigma} \qquad (4.9a)$$

$$PHP^{-1} = H \ \ , \ i.e. \ [P, H] = 0 \qquad (4.9b)$$

$$P\phi_i \ P^{-1} = \phi_{ip} \qquad (4.9c)$$

Using equation (4.9c) we can write the site-exchanged operators

$$\phi_{1p} = I_\theta \ c_{2\uparrow} = (1-n_{1\uparrow})(1-n_{1\downarrow})(1-n_{2\downarrow}) \ c_{2\uparrow}$$

$$\phi_{2p} = c_{2\downarrow}^\dagger \ I_\theta \ c_{2\downarrow} \ c_{2\uparrow} = (1-n_{1\uparrow})(1-n_{1\downarrow}) \ n_{2\downarrow} \ c_{2\uparrow}$$

$$\phi_{3p} = c_{1\uparrow}^\dagger \ I_\theta \ c_{1\uparrow} \ c_{2\uparrow} = (1-n_{1\downarrow})(1-n_{2\downarrow}) \ n_{1\uparrow} \ c_{2\uparrow}$$

$$\phi_{4p} = c_{1\downarrow}^\dagger \ I_\theta \ c_{1\downarrow} \ c_{2\uparrow} = (1-n_{1\uparrow})(1-n_{2\downarrow}) \ n_{1\downarrow} \ c_{2\uparrow}$$

$$\phi_{5p} = c_{2\downarrow}^\dagger \ c_{1\uparrow}^\dagger \ I_\theta \ c_{1\uparrow} \ c_{2\downarrow} \ c_{2\uparrow} = (1-n_{1\downarrow}) \ n_{2\downarrow} \ n_{1\uparrow} \ c_{2\uparrow}$$

$$\phi_{6p} = c_{2\downarrow}^\dagger \ c_{1\downarrow}^\dagger \ I_\theta \ c_{1\downarrow} \ c_{2\downarrow} \ c_{2\uparrow} = (1-n_{1\uparrow}) \ n_{2\downarrow} \ n_{1\downarrow} \ c_{2\uparrow}$$

$$\phi_{7p} = c_{1\uparrow}^{\dagger} c_{1\downarrow}^{\dagger} I_\theta c_{1\downarrow} c_{1\uparrow} c_{2\uparrow} = (1-n_{2\downarrow}) \, n_{1\downarrow} \, n_{1\uparrow} \, c_{2\uparrow}$$

$$\phi_{8p} = c_{2\downarrow}^{\dagger} c_{1\uparrow}^{\dagger} c_{1\downarrow}^{\dagger} I_\theta c_{1\downarrow} c_{1\uparrow} c_{2\downarrow} c_{2\uparrow} = n_{2\downarrow} \, n_{1\downarrow} \, n_{1\uparrow} \, c_{2\uparrow}$$

We will exploit the site-exchange symmetry of the Hamiltonian by constructing eigenvectors of L from site-exchanged pairs of ϕ's.

It will also be useful to introduce the following single-particle operators:

$$\tilde{\phi}_2 = c_{2\downarrow}^{\dagger} I_\theta c_{1\downarrow} c_{1\uparrow} = (1-n_{2\uparrow}) \, c_{2\downarrow}^{\dagger} c_{1\downarrow} c_{1\uparrow}$$

$$\tilde{\phi}_{2p} = c_{1\downarrow}^{\dagger} I_\theta c_{2\downarrow} c_{2\uparrow} = (1-n_{1\uparrow}) \, c_{1\downarrow}^{\dagger} c_{2\downarrow} c_{2\uparrow}$$

$$\tilde{\phi}_4 = c_{1\downarrow}^{\dagger} I_\theta c_{2\downarrow} c_{1\uparrow} = (1-n_{2\uparrow}) \, c_{1\downarrow}^{\dagger} c_{2\downarrow} c_{1\uparrow}$$

$$\tilde{\phi}_{4p} = c_{2\downarrow}^{\dagger} I_\theta c_{1\downarrow} c_{2\uparrow} = -(1-n_{1\uparrow}) \, c_{2\downarrow}^{\dagger} c_{2\uparrow} c_{1\downarrow}$$

$$\tilde{\phi}_5 = c_{1\downarrow}^{\dagger} c_{2\uparrow}^{\dagger} I_\theta c_{2\downarrow} c_{2\uparrow} c_{1\uparrow} = -n_{2\uparrow} \, c_{1\downarrow} c_{1\uparrow}$$

$$\tilde{\phi}_{5p} = c_{2\downarrow}^{\dagger} c_{1\uparrow}^{\dagger} I_\theta c_{1\downarrow} c_{1\uparrow} c_{2\uparrow} = n_{1\uparrow} \, c_{2\downarrow}^{\dagger} c_{2\uparrow} c_{1\downarrow}$$

$$\tilde{\phi}_7 = c_{2\uparrow}^{\dagger} c_{2\downarrow}^{\dagger} I_\theta c_{2\uparrow} c_{1\downarrow} c_{1\uparrow} = -n_{2\uparrow} \, c_{2\downarrow}^{\dagger} c_{1\downarrow} c_{1\uparrow}$$

$$\tilde{\phi}_{7p} = c_{1\uparrow}^{\dagger} c_{1\downarrow}^{\dagger} I_\theta c_{1\uparrow} c_{2\downarrow} c_{2\uparrow} = -n_{1\uparrow} \, c_{1\downarrow}^{\dagger} c_{2\downarrow} c_{2\uparrow}$$

The introduction of these operators is necessitated by the fact that the set of initial Judd operators ϕ_i and ϕ_{ip} (i = 1, 2,...,8) is not closed under the operation of the hopping part of the Liouville operator. This becomes evident as we look at the eigenvalue equation for the Liouville operator L, where, for any operator θ,

$$L\theta = L_o\theta + L_h\theta = [\theta, H_o] + [\theta, H_h] \tag{4.10a}$$

$$H_o = \sum_{i,\sigma} \varepsilon_{i,\sigma}\, n_{i,\sigma} + U\sum_i n_{i,\sigma}\, \bar{n}_{i,-\sigma} \tag{4.10b}$$

$$H_h = t\sum_\sigma (c_{1,\sigma}^\dagger c_{2,\sigma} + c_{2,\sigma}^\dagger c_{1,\sigma}) \tag{5.10c}$$

where ε is the electron "band" energy, U is the Coulomb energy between two electrons on the same atomic site, and t is the hopping energy between the two sites. We note that

$$L(ABC) = AB(LC) + A(LB)C + (LA)BC$$

and in particular

$$L_o c_{i,\sigma} = \varepsilon_{i,\sigma}\, c_{i,\sigma} + U n_{i,-\sigma}\, c_{i,\sigma}$$

$$L_o c_{i,\sigma}^\dagger = -\varepsilon_{i,\sigma}\, c_{i,\sigma}^\dagger - U n_{i\sigma}\, c_{i,\sigma}^\dagger$$

$$L_h c_{i,\sigma} = t c_{i\pm1,\sigma}$$

$$L_h c_{i,\sigma}^\dagger = -t c_{i\pm1,\sigma}^\dagger$$

$$L_o n_{i,\sigma} = 0$$

$$L_h n_{i,\sigma} = t(c_{i,\sigma}^\dagger c_{i\pm1,\sigma} - c_{i\pm1,\sigma}^\dagger c_{i,\sigma}) \ .$$

We make the assumption that $\varepsilon_{1,\sigma} = \varepsilon_{2,\sigma} = \varepsilon_\sigma$ which is a statement of translational invariance. We also have $\varepsilon_\sigma = \varepsilon$ for no external magnetic fields. Note further that $L_o I_\theta = L_h I_\theta = 0$.

The next step in our calculation is to write out explicitly the operation of the Liouville operator on the set of twenty-four single-

particle Judd operators which we have amassed:

$$L_o \phi_1 = \varepsilon\, \phi_1 \qquad\qquad L_o \phi_{1p} = \varepsilon\, \phi_{1p}$$

$$L_o \phi_2 = (\varepsilon + U)\, \phi_2 \qquad\qquad L_o \phi_{2p} = (\varepsilon + U)\, \phi_{2p}$$

$$L_o \phi_3 = \varepsilon\, \phi_3 \qquad\qquad L_o \phi_{3p} = \varepsilon\, \phi_{3p}$$

$$L_o \phi_4 = \varepsilon\, \phi_4 \qquad\qquad L_o \phi_{4p} = \varepsilon\, \phi_{4p}$$

$$L_o \phi_5 = (\varepsilon + U)\, \phi_5 \qquad\qquad L_o \phi_{5p} = (\varepsilon + U)\, \phi_{5p}$$

$$L_o \phi_6 = (\varepsilon + U)\, \phi_6 \qquad\qquad L_o \phi_{6p} = (\varepsilon + U)\, \phi_{6p}$$

$$L_o \phi_7 = \varepsilon\, \phi_7 \qquad\qquad L_o \phi_{7p} = \varepsilon\, \phi_{7p}$$

$$L_o \phi_8 = (\varepsilon + U)\, \phi_8 \qquad\qquad L_o \phi_{8p} = (\varepsilon + U)\, \phi_{8p}$$

$$L_o \tilde{\phi}_2 = (\varepsilon + U)\, \tilde{\phi}_2 \qquad\qquad L_o \tilde{\phi}_{2p} = (\varepsilon + U)\, \tilde{\phi}_{2p}$$

$$L_o \tilde{\phi}_4 = \varepsilon\, \tilde{\phi}_4 \qquad\qquad L_o \tilde{\phi}_{4p} = \varepsilon\, \tilde{\phi}_{4p}$$

$$L_o \tilde{\phi}_5 = (\varepsilon + U)\, \tilde{\phi}_5 \qquad\qquad L_o \tilde{\phi}_{5p} = (\varepsilon + U)\, \tilde{\phi}_{5p}$$

$$L_o \tilde{\phi}_7 = \varepsilon\, \tilde{\phi}_7 \qquad\qquad L_o \tilde{\phi}_{7p} = \varepsilon\, \tilde{\phi}_{7p}$$

$$L_h \phi_1 = t\, \phi_{1p} \qquad\qquad L_h \phi_{1p} = t\, \phi_1$$

$$L_h \phi_2 = t\, (\phi_{4p} + \tilde{\phi}_4 - \tilde{\phi}_2) \qquad\qquad L_h \phi_{2p} = t\, (\phi_4 + \tilde{\phi}_{4p} - \tilde{\phi}_{2p})$$

$$L_h \phi_3 = t\, \phi_{3p} \qquad\qquad L_h \phi_{3p} = t\, \phi_3$$

$$L_h \phi_4 = t\, (\phi_{2p} + \tilde{\phi}_2 - \tilde{\phi}_4) \qquad\qquad L_h \phi_{4p} = t\, (\phi_2 + \tilde{\phi}_{2p} - \tilde{\phi}_{4p})$$

$$L_h \phi_5 = t \, (-\tilde{\phi}_5 + \phi_{7p} + \tilde{\phi}_7)$$

$$L_h \phi_{5p} = t \, (\phi_7 + \tilde{\phi}_{7p} - \tilde{\phi}_{5p})$$

$$L_h \phi_6 = t \, \phi_{6p}$$

$$L_h \phi_{6p} = t \, \phi_6$$

$$L_h \phi_7 = t \, (-\tilde{\phi}_7 + \tilde{\phi}_5 + \phi_{5p})$$

$$L_h \phi_{7p} = t \, (\phi_5 + \tilde{\phi}_{5p} - \tilde{\phi}_{7p})$$

$$L_h \phi_8 = t \, \phi_{8p}$$

$$L_h \phi_{8p} = t \, \phi_8$$

$$L_h \tilde{\phi}_2 = t \, (\tilde{\phi}_{4p} + \phi_4 - \phi_2)$$

$$L_h \tilde{\phi}_{2p} = t \, (\tilde{\phi}_4 + \phi_4 - \phi_{2p})$$

$$L_h \tilde{\phi}_4 = t \, (\tilde{\phi}_{2p} + \phi_2 - \phi_4)$$

$$L_h \tilde{\phi}_{4p} = t \, (\tilde{\phi}_2 + \phi_{2p} - \phi_{4p})$$

$$L_h \tilde{\phi}_5 = t \, (\phi_7 - \phi_5 + \tilde{\phi}_{7p})$$

$$L_h \tilde{\phi}_{5p} = t \, (\phi_{7p} - \phi_{5p} + \tilde{\phi}_7)$$

$$L_h \tilde{\phi}_7 = t \, (\phi_5 - \phi_7 + \tilde{\phi}_{5p})$$

$$L_h \tilde{\phi}_{7p} = t \, (\phi_{5p} - \phi_{7p} + \tilde{\phi}_5)$$

Using these twenty-four Judd states, we wish to construct the corresponding twenty-four eigenstates of the Liouville operator. Taking advantage of the site-exchange symmetry of the Hamiltonian we may immediately write down sixteen of the eigenstates:

$$\psi_{1\pm} = \phi_{1\pm} = I_\theta \, (c_{1\uparrow} \pm c_{2\uparrow})$$

$$\psi_{2\pm} = \phi_{2\pm} \mp \tilde{\phi}_{2\pm} = (c_{1\downarrow}^\dagger \mp c_{2\downarrow}^\dagger) \, I_\theta \, (c_{1\downarrow} \, c_{1\uparrow} - c_{2\downarrow} \, c_{2\uparrow})$$

$$\psi_{3\pm} = \phi_{3\pm} = (c_{2\uparrow}^\dagger \mp c_{1\uparrow}^\dagger) \, I_\theta \, c_{2\uparrow} \, c_{1\uparrow}$$

$$\psi_{4\pm} = \phi_{4\pm} \mp \tilde{\phi}_{4\pm} = (c_{1\downarrow}^\dagger \mp c_{2\downarrow}^\dagger) \, I_\theta \, (c_{1\downarrow} \, c_{2\uparrow} - c_{2\downarrow} \, c_{1\uparrow})$$

$$\psi_{5\pm} = \phi_{5\pm} \mp \tilde{\phi}_{5\pm} = (c_{1\downarrow}^\dagger \, c_{2\uparrow}^\dagger - c_{2\downarrow}^\dagger \, c_{1\uparrow}^\dagger) \, I_\theta \, (c_{2\uparrow} \, c_{1\downarrow} \, c_{1\uparrow} \mp c_{2\downarrow} \, c_{2\uparrow} \, c_{1\uparrow})$$

$$\psi_{6\pm} = \phi_{6\pm} = c_{1\downarrow}^\dagger \, c_{2\downarrow}^\dagger \, I_\theta \, (c_{2\downarrow} \, c_{1\downarrow} \, c_{1\uparrow} \mp c_{2\downarrow} \, c_{2\uparrow} \, c_{1\downarrow})$$

$$\psi_{7\pm} = \phi_{7\pm} \mp \tilde{\phi}_{7\pm} = (c_{2\uparrow}^\dagger c_{2\downarrow}^\dagger - c_{1\uparrow}^\dagger c_{1\downarrow}^\dagger) \, I_\theta \, (c_{2\downarrow} c_{2\uparrow} c_{1\uparrow} \mp c_{2\uparrow} c_{1\downarrow} c_{1\uparrow})$$

$$\psi_{8\pm} = \phi_{8\pm} = (c_{1\downarrow}^\dagger c_{2\uparrow}^\dagger c_{2\downarrow}^\dagger \pm c_{2\downarrow}^\dagger c_{1\uparrow}^\dagger c_{1\downarrow}^\dagger) \, I_\theta \, c_{2\downarrow} c_{2\uparrow} c_{1\downarrow} c_{1\uparrow}$$

where we define $\phi_{i\pm} = \phi_i \pm \phi_{ip}$. These sixteen eigenstates obey the following eigenvalue equations:

$$L\psi_{1\pm} = (\varepsilon \pm t) \, \psi_{1\pm}$$

$$L\psi_{2\pm} = (\varepsilon + U \pm t) \, \psi_{2\pm}$$

$$L\psi_{3\pm} = (\varepsilon \pm t) \, \psi_{3\pm}$$

$$L\psi_{4\pm} = (\varepsilon \pm t) \, \psi_{4\pm}$$

$$L\psi_{5\pm} = (\varepsilon + U \pm t) \, \psi_{5\pm}$$

$$L\psi_{6\pm} = (\varepsilon + U \pm t) \, \psi_{6\pm}$$

$$L\psi_{7\pm} = (\varepsilon \pm t) \, \psi_{7\pm}$$

$$L\psi_{8\pm} = (\varepsilon + U \pm t) \, \psi_{8\pm}$$

The remaining eight eigenstates may be constructed by taking appropriate linear combinations of site-exchanged pairs. Then by diagonalizing four 2 x 2 matrices by standard techniques, we obtain expressions for the remaining eight eigenstates of L:

$$\psi_{2\pm}^{(1)} = \alpha_1 \, (\phi_{2\pm} \pm \tilde{\phi}_{2\pm}) \mp \beta_1 \, (\phi_{4\pm} \pm \tilde{\phi}_{4\pm})$$

$$= (c_{1\downarrow}^\dagger \pm c_{2\downarrow}^\dagger) \, I_\theta \, [\alpha_1 \, (c_{1\downarrow} c_{1\uparrow} + c_{2\downarrow} c_{2\uparrow}) + \beta_1 (c_{1\downarrow} c_{2\uparrow} + c_{2\downarrow} c_{1\uparrow})]$$

$$\psi_{2\pm}^{(2)} = \alpha_2 \, (\phi_{2\pm} \pm \tilde{\phi}_{2\pm}) \pm \beta_2 \, (\phi_{4\pm} \mp \tilde{\phi}_{4\pm})$$

$$= (c_{1\downarrow}^\dagger \pm c_{2\downarrow}^\dagger) \, I_\theta \, [\alpha_2 \, (c_{1\downarrow} \, c_{1\uparrow} + c_{2\downarrow} \, c_{2\uparrow}) + \beta_2 \, (c_{1\downarrow} \, c_{2\uparrow} + c_{2\downarrow} \, c_{1\uparrow})]$$

$$\psi_{5\pm}^{(1)} = \alpha_1 \, (\phi_{5\pm} \pm \tilde{\phi}_{5\pm}) \pm \beta_1 \, (\phi_{7\pm} \mp \tilde{\phi}_{7\pm})$$

$$= [\alpha_1 \, (c_{1\downarrow}^\dagger \, c_{2\uparrow}^\dagger + c_{2\downarrow}^\dagger \, c_{1\uparrow}^\dagger) + \beta_1 \, (c_{1\uparrow}^\dagger \, c_{1\downarrow}^\dagger + c_{2\uparrow}^\dagger \, c_{2\downarrow}^\dagger)] \, I_\theta \; x$$

$$(c_{2\downarrow} \, c_{2\uparrow} \, c_{1\uparrow} \pm c_{2\uparrow} \, c_{1\downarrow} \, c_{1\uparrow})$$

$$\psi_{5\pm}^{(2)} = \alpha_2 \, (\phi_{5\pm} \pm \tilde{\phi}_{5\pm}) \pm \beta_2 \, (\phi_{7\pm} \pm \tilde{\phi}_{7\pm})$$

$$= [\beta_2 \, (c_{1\uparrow}^\dagger \, c_{1\downarrow}^\dagger + c_{2\uparrow}^\dagger \, c_{2\downarrow}^\dagger) - \alpha_2 \, (c_{2\uparrow}^\dagger \, c_{1\downarrow}^\dagger + c_{1\uparrow}^\dagger \, c_{2\downarrow}^\dagger)] \, I_\theta \; x$$

$$(c_{2\downarrow} \, c_{2\uparrow} \, c_{1\uparrow} \pm c_{2\uparrow} \, c_{1\downarrow} \, c_{1\uparrow}) \quad .$$

The corresponding eigenvalue equations are

$$L\psi_{2\pm}^{(1)} = \lambda_{1\pm} \, \psi_{2\pm}^{(1)}$$

$$L\psi_{2\pm}^{(2)} = \lambda_{2\pm} \, \psi_{2\pm}^{(2)}$$

$$L\psi_{5\pm}^{(1)} = \lambda_{1\pm} \, \psi_{5\pm}^{(1)}$$

$$L\psi_{5\pm}^{(2)} = \lambda_{2\pm} \, \psi_{5\pm}^{(2)}$$

where we define

$$\alpha_1 = \frac{1}{D_1} \, [\tfrac{1}{2}U - (\tfrac{1}{4}U^2 + 4t^2)^{\frac{1}{2}}] \, , \quad \alpha_2 = \frac{1}{D_2} \, [\tfrac{1}{2}U + (\tfrac{1}{4}U^2 + 4t^2)^{\frac{1}{2}}]$$

$$\beta_1 = 2t/D_1 \quad , \quad \beta_2 = 2t/D_2$$

$$D_1 = \frac{1}{\sqrt{2}} \, [U^2 + 16t^2 - U(U^2 + 16t^2)^{\frac{1}{2}}]^{\frac{1}{2}}$$

$$D_2 = \frac{1}{\sqrt{2}} \, [U^2 + 16t^2 + U(U^2 + 16t^2)^{\frac{1}{2}}]^{\frac{1}{2}}$$

$$\alpha_1\beta_1 = -\alpha_2\beta_2 = \frac{-2t}{(U^2 + 16t^2)^{\frac{1}{2}}}$$

$$\lambda_{1\pm} = \varepsilon + \frac{1}{2}U \mp t - (\frac{1}{4}U^2 + 4t^2)^{\frac{1}{2}}$$

$$\lambda_{2\pm} = \varepsilon + \frac{1}{2}U \mp t + (\frac{1}{4}U^2 + 4t^2)^{\frac{1}{2}}$$

We have now constructed a complete set of orthogonal eigenstates of the Liouville operator for the Hubbard s-band dimer. The use of the word complete warrants some discussion. Our efforts to this point have been directed towards the calculation of the single-particle Green function

$$G_{1\uparrow}(\omega) = ((c_{1\uparrow}, (\omega-L)^{-1} c_{1\uparrow})) \quad . \tag{4.11}$$

Using site exchange invariance, we see that this is equivalent to the calculation of

$$G_{2\uparrow}(\omega) = ((c_{2\uparrow}, (\omega-L)^{-1} c_{2\uparrow})) \quad .$$

The region of superspace spanned in these two calculations is therefore the same. Hence the twenty-four Judd operators which we have been dealing with comprise a subspace of the Hubbard s-band dimer single-particle superspace. This single-particle superspace is in turn a subspace of the entire Hubbard s-band dimer fermion superspace involving three-particle operators as well as one-particle operators. From the Lie algebra analysis we also know that the superspace contains operators which keep the number of particles constant while stepping between different spin states.

Had we chosen at the outset to investigate the single-particle Green function

$$G_{1\downarrow}(\omega) = ((c_{1\downarrow}, (\omega-L)^{-1} c_{1\downarrow}))$$

or equivalently

$$G_{2\downarrow}(\omega) = ((c_{2\downarrow}, (\omega-L)^{-1} c_{2\downarrow})) \quad ,$$

we would have had to introduce the spin-flipped set of twenty-four Judd operators. The entire single-particle Hubbard s-band dimer fermion superspace must therefore contain at least forty-eight elements. In Appendix (A) we show that there are four remaining site-exchanged pairs of single-particle operators. These "anomalous" single-particle operators step between states which differ in spin by 3/2. That is, although there is a single particle being destroyed as required, there is at the same time a different particle which is flipping spin. These operators do not play a role in our model on the physical basis that there are no spin-flip terms in our Hamiltonian and there are no externally applied magnetic fields. We see therefore that the complete single-particle fermion superspace for the Hubbard dimer contains fifty-six elements, twenty-four of which we use in the calculation of the Green function

$$G_{1\uparrow}(\omega) = ((c_{1\uparrow}, (\omega-L)^{-1} c_{1\uparrow})) \quad .$$

It is clear that the size of the subspace needed for calculation depends on the nature of the Hamiltonian. For example, adding a

magnetic interaction and a spin-flip interaction to our Hamiltonian would increase the number of single-particle operators to the full fifty-six, thus eliminating much of the degeneracy of the states. In summary then, the size of the superspace needed depends on the physics of the problem, i.e., on the Hamiltonian.

Having completed the construction of the single-particle eigenstates of the Liouville operator,

$$L\psi_1 = \lambda_i \psi_i \, ,$$

we wish to re-express the operator $c_{1\uparrow}$ in terms of these eigenstates. This is accomplished by using the relations

$$\phi_i = \frac{1}{2}(\phi_{i+} + \phi_{i-}) = \frac{1}{2}(\psi_{i+} + \psi_{i-}), \quad i = 1, 3, 6, 8$$

$$\phi_k = \frac{1}{4}[\psi_{k+} + \psi_{k-} + \beta_1(\psi_{k+}^{(2)} + \psi_{k-}^{(2)}) - \beta_2(\psi_{k+}^{(1)} + \psi_{k-}^{(1)})]$$

$$\phi_\ell = \frac{1}{4}[\psi_{\ell+} + \psi_{\ell-} + \alpha_2(\psi_{k+}^{(1)} - \psi_{k-}^{(1)}) - \alpha_1(\psi_{k+}^{(2)} - \psi_{k-}^{(1)})]$$

where $k = 2,5$ and $\ell = k + 2$. A straightforward substitution in equation (4.8) yields the explicit result

$$c_{1\uparrow} = \frac{1}{2}[\psi_{1+} + \psi_{1-} + \psi_{3+} + \psi_{3-} + \psi_{6+} + \psi_{6-} + \psi_{8+} + \psi_{8-}$$

$$+ \frac{1}{2}[\psi_{2+} + \psi_{2-} + \psi_{4+} + \psi_{4-} + \psi_{5+} + \psi_{5-} + \psi_{7+} + \psi_{7-}$$

$$+ \beta_1(\psi_{2+}^{(2)} + \psi_{2-}^{(2)} + \psi_{5+}^{(2)} + \psi_{5-}^{(2)})$$

$$- \beta_2(\psi_{2+}^{(1)} + \psi_{2-}^{(1)} + \psi_{5+}^{(1)} + \psi_{5-}^{(1)})$$

$$+ \alpha_2(\psi_{2+}^{(1)} - \psi_{2-}^{(1)} + \psi_{5+}^{(1)} - \psi_{5-}^{(1)})$$

$$- \alpha_1 (\psi_{2+}^{(2)} - \psi_{2-}^{(2)} + \psi_{5+}^{(2)} - \psi_{5-}^{(2)})] \} \quad .$$

The single-particle Green function is then given by

$$G_{1\uparrow}(\omega) = ((c_{1\uparrow}, \ (\omega-L)^{-1} \ c_{1\uparrow}))$$

$$= \frac{1}{16} \ \{ [4((\psi_{1+}, \ \psi_{1+})) + 4((\psi_{3+}, \ \psi_{3+})) + ((\psi_{4+}, \ \psi_{4+})) +$$

$$((\psi_{7+}, \ \psi_{7+}))] \ \frac{1}{\omega - (\varepsilon+t)}$$

$$+ [4((\psi_{1-}, \ \psi_{1-})) + 4((\psi_{3-}, \ \psi_{3-})) + ((\psi_{4-}, \ \psi_{4-})) +$$

$$((\psi_{7-}, \ \psi_{7-}))] \ \frac{1}{\omega - (\varepsilon-t)}$$

$$+ [((\psi_{2+}, \ \psi_{2+})) + ((\psi_{5+}, \ \psi_{5+})) + 4((\psi_{6+}, \ \psi_{6+})) +$$

$$+ 4((\psi_{8+}, \ \psi_{8+}))] \ \frac{1}{\omega - (\varepsilon + U + t)}$$

$$+ [((\psi_{2-}, \ \psi_{2-})) + ((\psi_{5-}, \ \psi_{5-})) + 4((\psi_{6-}, \ \psi_{6-})) +$$

$$4((\psi_{8-}, \ \psi_{8-}))] \ \frac{1}{\omega - (\varepsilon + U - t)}$$

$$+ (1-2\alpha_2\beta_2) \ [((\psi_{2+}, \ \psi_{2+}^{(1)})) + ((\psi_{5+}, \ \psi_{5+}^{(1)}))] \ x$$

$$\frac{1}{\omega - (\varepsilon + \tfrac{1}{2}U - t - (\tfrac{1}{4}U^2 + 4t^2)^{\frac{1}{2}})}$$

$$+ (1+2\alpha_2\beta_2) \ [((\psi_{2-}, \ \psi_{2-}^{(1)})) + ((\psi_{5-}, \ \psi_{5-}^{(1)}))] \ x$$

$$\frac{1}{\omega - (\varepsilon + \tfrac{1}{2}U + t - (\tfrac{1}{4}U^2 + 4t^2)^{\frac{1}{2}})}$$

$$+ (1-2\alpha_1\beta_1) [((\psi_{2+}^{(2)}, \psi_{2+}^{(2)})) + ((\psi_{5+}^{(2)}, \psi_{5+}^{(2)}))] \text{ x}$$

$$\frac{1}{\omega - (\epsilon + \tfrac{1}{2}U - t + (\tfrac{1}{4}U^2 + 4t^2)^{\frac{1}{2}})}$$

$$+ (1+2\alpha_1\beta_1) [((\psi_{2-}^{(2)}, \psi_{2-}^{(2)})) + ((\psi_{5-}^{(2)}, \psi_{5-}^{(2)}))] \text{ x}$$

$$\frac{1}{\omega - (\epsilon + \tfrac{1}{2}U + t + (\tfrac{1}{4}U^2 + 4t^2)^{\frac{1}{2}})} \} .$$

$$(4.13)$$

In appendix (B) we solve for the inner products $((\psi_{i\pm}, \psi_{i\pm}))$ in terms of the correlation functions:

$$X1 = \langle n_{1\uparrow} \rangle = \langle n_{1\downarrow} \rangle = \langle n_{2\uparrow} \rangle = \langle n_{2\downarrow} \rangle$$

$$X2 = \langle n_{1\uparrow} n_{2\uparrow} \rangle = \langle n_{1\downarrow} n_{2\downarrow} \rangle$$

$$X3 = \langle n_{1\uparrow} n_{1\downarrow} \rangle = \langle n_{2\uparrow} n_{2\downarrow} \rangle$$

$$X4 = \langle n_{1\uparrow} n_{2\downarrow} \rangle = \langle n_{2\uparrow} n_{1\downarrow} \rangle$$

$$X5 = \langle n_{1\uparrow} n_{1\downarrow} n_{2\uparrow} \rangle = \langle n_{1\uparrow} n_{1\downarrow} n_{2\downarrow} \rangle = \langle n_{2\uparrow} n_{2\downarrow} n_{1\uparrow} \rangle = \langle n_{2\uparrow} n_{2\downarrow} n_{1\downarrow} \rangle$$

$$X6 = \langle n_{1\uparrow} n_{1\downarrow} n_{2\uparrow} n_{2\downarrow} \rangle$$

$$X7 = \langle c_{1\uparrow}^\dagger c_{2\uparrow} \rangle = \langle c_{2\uparrow}^\dagger c_{1\uparrow} \rangle = \langle c_{1\downarrow}^\dagger c_{2\downarrow} \rangle = \langle c_{2\downarrow}^\dagger c_{1\downarrow} \rangle$$

$$X8 = \langle n_{1\downarrow} c_{1\uparrow}^\dagger c_{2\uparrow} \rangle = \langle n_{2\downarrow} c_{2\uparrow}^\dagger c_{1\uparrow} \rangle = \langle n_{1\uparrow} c_{1\downarrow}^\dagger c_{2\downarrow} \rangle = \langle n_{2\uparrow} c_{2\downarrow}^\dagger c_{1\downarrow} \rangle$$

$$X9 = \langle n_{2\downarrow} c_{1\uparrow}^\dagger c_{2\uparrow} \rangle = \langle n_{1\downarrow} c_{2\uparrow}^\dagger c_{1\uparrow} \rangle = \langle n_{2\uparrow} c_{1\downarrow}^\dagger c_{2\downarrow} \rangle = \langle n_{1\uparrow} c_{2\downarrow}^\dagger c_{1\downarrow} \rangle$$

$$X10 = <n_{1\uparrow} \, n_{1\downarrow} \, c_{2\uparrow}^{\dagger} \, c_{2\downarrow}> = <n_{1\uparrow} \, n_{1\downarrow} \, c_{2\downarrow}^{\dagger} \, c_{2\uparrow}> = <n_{2\uparrow} \, n_{2\downarrow}^{\dagger} \, c_{1\uparrow} \, c_{1\downarrow}> =$$

$$<n_{2\uparrow} \, n_{2\downarrow} \, c_{1\downarrow}^{\dagger} \, c_{1\uparrow}>$$

$$X11 = <c_{1\downarrow}^{\dagger} \, c_{2\downarrow} \, c_{1\uparrow}^{\dagger} \, c_{2\uparrow}> = <c_{2\downarrow}^{\dagger} \, c_{1\downarrow} \, c_{2\uparrow}^{\dagger} \, c_{1\uparrow}>$$

$$X12 = <c_{1\downarrow}^{\dagger} \, c_{2\downarrow} \, c_{2\uparrow}^{\dagger} \, c_{1\uparrow}> = <c_{2\downarrow}^{\dagger} \, c_{1\downarrow} \, c_{1\uparrow}^{\dagger} \, c_{2\uparrow}> \quad .$$

This set of correlation functions is solved for by using the dispersion relations

$$<\psi_{i}^{\dagger} \, \psi_{i}> = ((\psi_{i}, \, \psi_{i})) \, f_{0} \, (\lambda_{i}),$$

where $L\psi_{i} = \lambda_{i} \, \psi_{i}$ and $f_{0}(\lambda_{i}) = (e^{\beta(\lambda_{i}-\mu)} + 1)^{-1}$.

It should be pointed out that the set of twenty-four dispersion relations obtained by evaluating the diagonal single-particle Green function is not sufficient to solve for the twelve correlation functions. Additional independent equations were obtained from an orthogonality relation and from the dispersion relation arising from the off-diagonal Green-function:

$$G_{1\uparrow, 2\uparrow} = ((c_{1\uparrow}, \, (\omega-L)^{-1} \, c_{2\uparrow})) \quad .$$

We list the set of equations obtained in appendix C. Included in this set is the dispersion relation obtained from $<n_{i,\sigma}> = <c_{i,\sigma}^{\dagger} \, c_{i,\sigma}>$.

V. RESULTS AND CONCLUSIONS

In the preceding chapters we have introduced a new method of calculation whereby the eigenvalue equation of the Liouville operator, L, as opposed to the Hamiltonian operator, H, was used. It should be pointed out that the two schemes are not unrelated. The eigenvalues of the Liouville operator correspond to differences in eigenvalues of the Hamiltonian operator.[41] A proof of this statement is the following. A typical eigenvalue equation for the Liouville operator is given by

$$L\psi_i^{(n \to m)} = \lambda_i^{(n \to m)} \psi_i^{(n \to m)}$$

where $\psi_i^{(n \to m)}$ is a vector in the superspace and a stepping operator between n- and m-particle states in Fock space. We now take this operator equation and operate on an n-particle energy eigenstate in Fock space given by $|\varepsilon_n\rangle$ (in Dirac bra-ket notation):

$$L\psi_i^{(n \to m)} |\varepsilon_n\rangle = [\psi_i^{(n \to m)} , H] |\varepsilon_n\rangle = \lambda_i^{(n \to m)} \psi_i^{(n \to m)} |\varepsilon_n\rangle \qquad (5.2a)$$

$$\varepsilon_n \psi_i^{(n \to m)} |\varepsilon_n\rangle - H\psi_i^{(n \to m)} |\varepsilon_n\rangle = \lambda_i^{(n \to m)} \psi_i^{(n \to m)} |\varepsilon_n\rangle . \qquad (5.2b)$$

We define the m-particle Fock space state

$$|\xi_m^i\rangle = \psi_i^{(n \to m)} |\varepsilon_n\rangle \quad .$$

Equation (5.2b) becomes

$$\varepsilon_n |\xi_m^i\rangle - H|\xi_m^i\rangle = \lambda_i^{(n \to m)} |\xi_m^i\rangle \quad ,$$

which upon rearrangement gives

$$H|\xi_m^i\rangle = (\varepsilon_n - \lambda_i^{(n\to m)})|\xi_m^i\rangle \quad . \tag{5.3}$$

It then follows (when $|\xi_m^i\rangle \neq 0$) that

$$|\xi_m^i\rangle = |\varepsilon_{m,i}\rangle \quad ,$$

i.e. the state $|\xi_m^i\rangle$ is an m-particle eigenstate of the Hamiltonian and also $\lambda_i^{(n\to m)} = \varepsilon_n - \varepsilon_{m,i}'$. That is, an eigenvalue of the Liouville operator for an eigenstate which is an (n→m)-particle stepping operator may be expressed as a difference of n- and m-particle eigenvalues of the Hamiltonian operator.

We can see therefore that solving a problem by diagonalizing the Liouville operator is equivalent to working with a diagonalized Hamiltonian operator. This equivalence is further illustrated in the structure of the eigenfunctions of L. As has been noted previously the relevant eigenfunctions of the Liouville operator, $\psi_i^{(n\to n-1)}$, are single-particle stepping operators in the superspace. It may also be shown[42] that each $\psi_i^{(n\to n-1)}$ must have the Judd structure $\psi_i^{(n\to n-1)} = A_{i,n-1}^\dagger \, I \, A_{i,n}'$, where $A_{i,n}'$ destroys an n-particle energy eigenstate in Fock space and $A_{i,n-1}^\dagger$ creates an (n-1)-particle energy eigenstate in Fock space. Thus by grouping the eigenfunctions $\psi_i^{(n\to n-1)}$ stepping to the known (n-1)-particle ground state and picking out the one with the smallest eigenvalue $\lambda_i^{(n\to n-1)}$, we are simultaneously choosing that eigenfunction of L which corresponds to a transition between ground-state to ground-state eigenfunctions of the Hamiltonian. For the 1→0 transition ψ_{1-} has the lowest eigenvalue, $\varepsilon - t$, with ψ_{1-} given by

$$\psi_{1-} = I_\theta \ (c_{1\uparrow} - c_{2\uparrow}) \quad .$$

This ψ steps to the known zero-particle (zero-energy) ground state

$$|00\rangle|00\rangle$$

in the notation $|n_{1\uparrow} \ n_{1\downarrow}\rangle|n_{2\uparrow} \ n_{2\downarrow}\rangle$ where 1, 2 refer to the sites in the dimer and $\uparrow$, $\downarrow$ refers to the spin. Thus, the single-particle ground state is $\frac{1}{\sqrt{2}} \ (|10\rangle|00\rangle - |00\rangle|10\rangle)$. By similiar reasoning the two-particle, three-particle and four-particle ground-state eigenfunctions of the Hamiltonian are obtained from $\psi_{2-}^{(1)}$, $\psi_{5+}^{(2)}$ and ψ_{8+} respectively (see Ref. 14 for comparison).

In Chapter IV we obtained the solution for the Hubbard dimer. That is, the single-particle Green function

$$G_{1\uparrow}(\omega) = ((c_{1\uparrow}, \ (\omega-L)^{-1} c_{1\uparrow}))$$

was evaluated exactly as was a set of twelve correlation functions, using the Judd operator formalism. It is the purpose of this chapter to investigate the calculated results for these correlation functions for various rations of t/U, where t is the hopping energy and U is the intra-site Coulomb energy, and for different values of the chemical potential. In the following analysis we have chosen $\varepsilon = 0$ and $U = 1$ eV. Therefore, the three parameters we have elected to vary are the hopping energy t, the chemical potential μ, and the temperature T.

In Figure 1 we plot the correlation function X1 as a function of chemical potential. Prior to our Judd operator calculations this plot had not been presented elsewhere. The reason for this is that most

PLOT OF X1 FOR t/U=.2

t/KT=5.79

1.159

0.232

<N>

CHEMICAL POTENTIAL
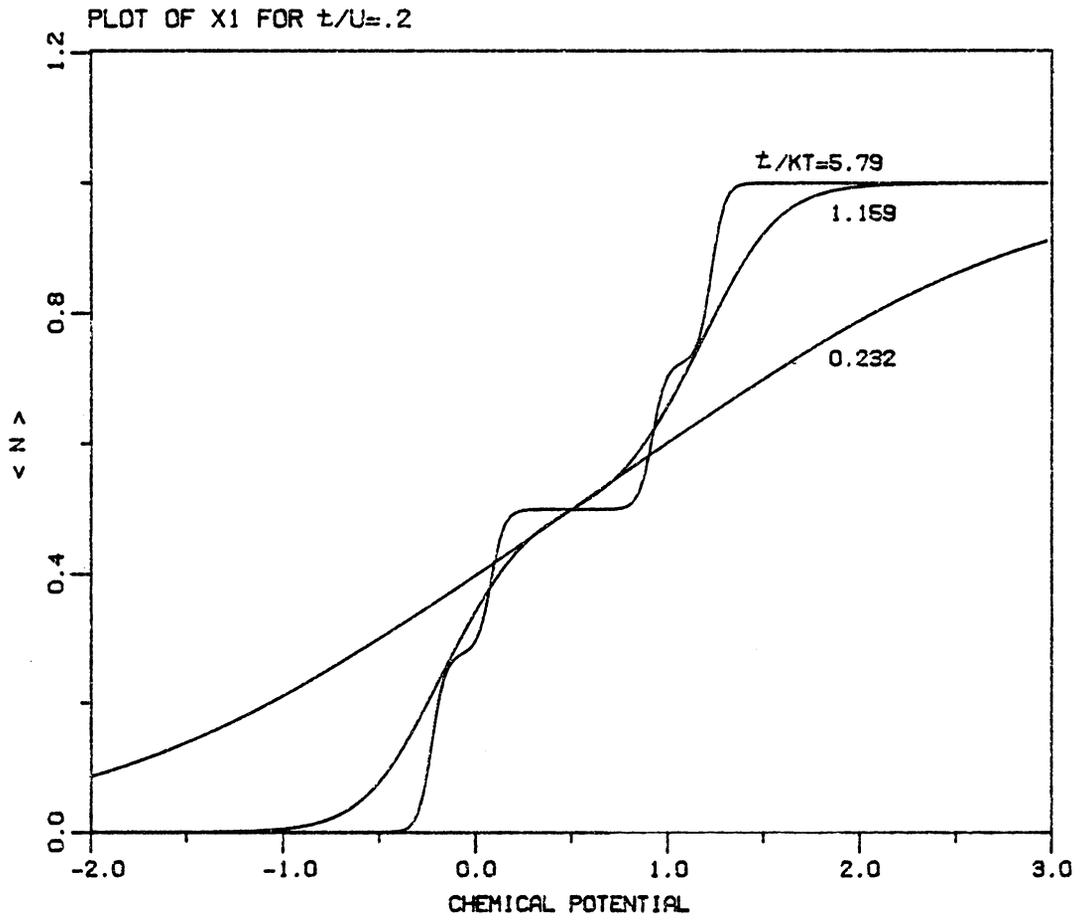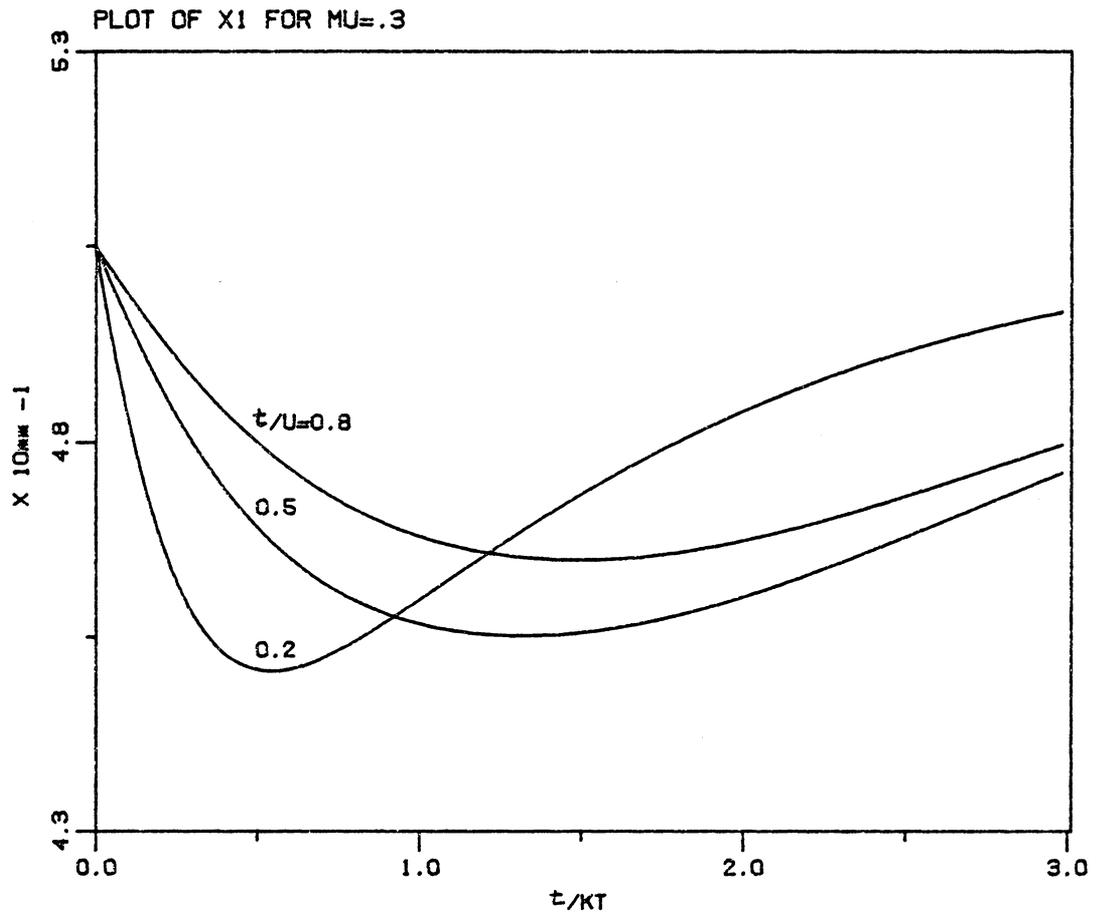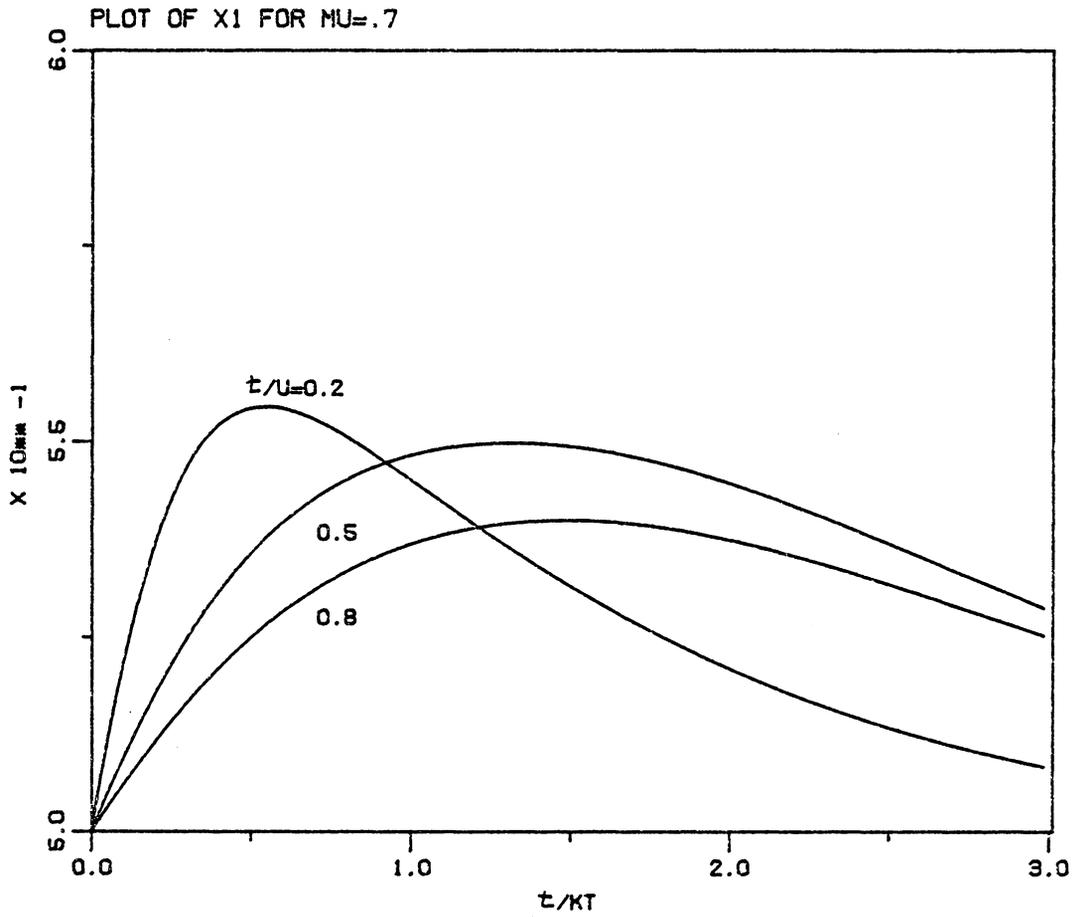
FIGURE 1.

FIGURE 2.

FIGURE 3.

FIGURE 4.

FIGURE 5.

PLOT OF X2 FOR MU=.7

FIGURE 6.

FIGURE 7.

PLOT OF X3 FOR MU=.489
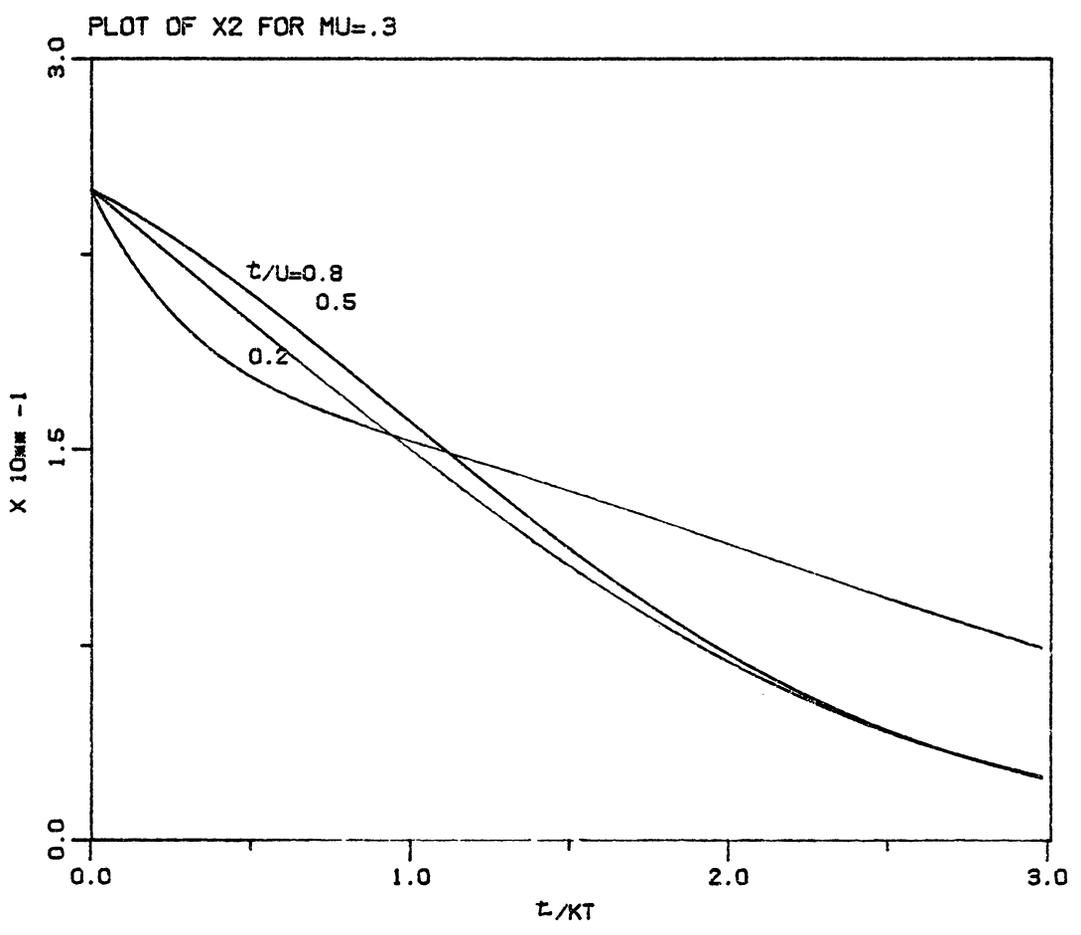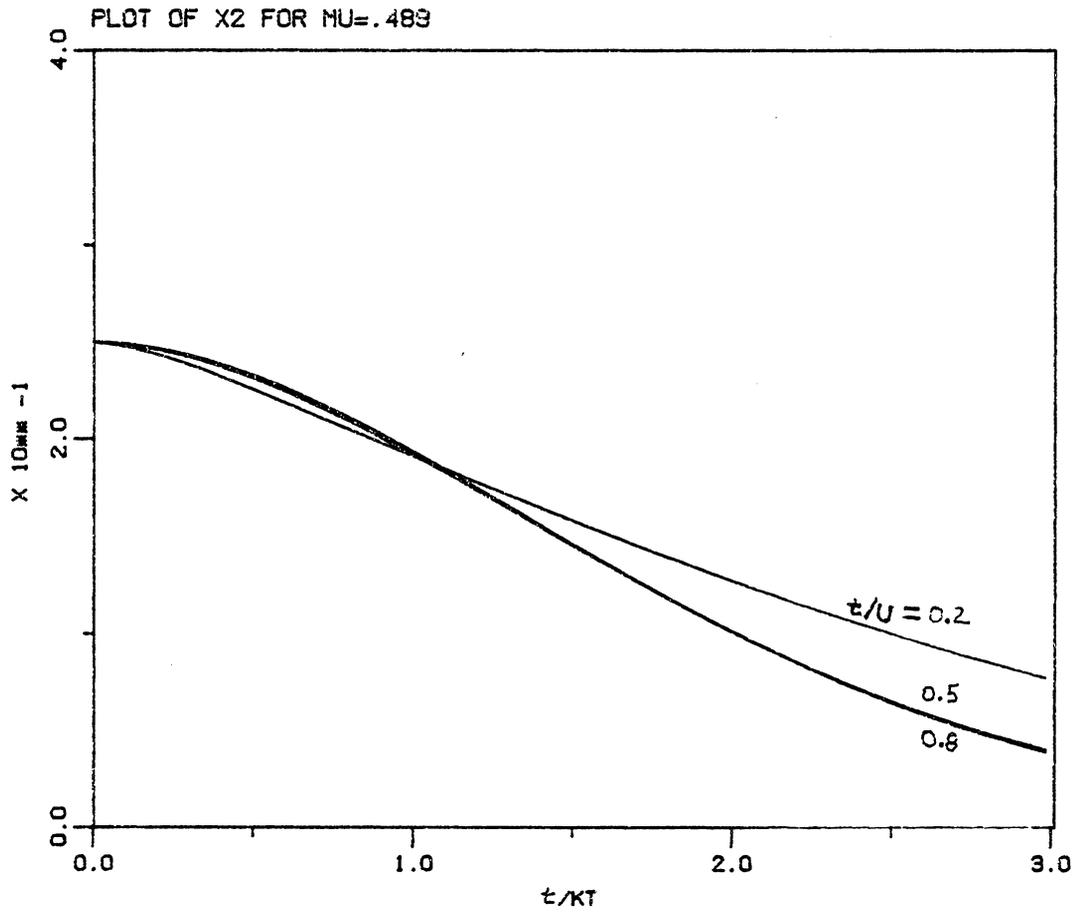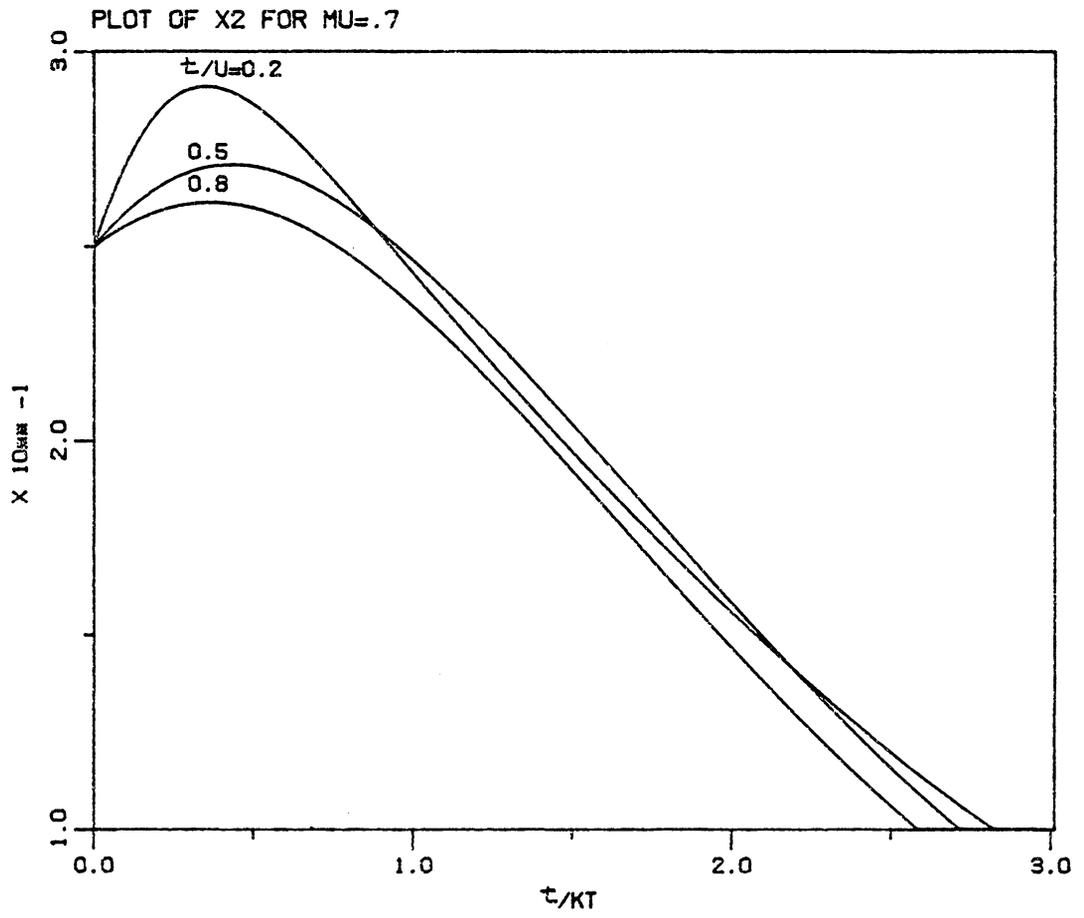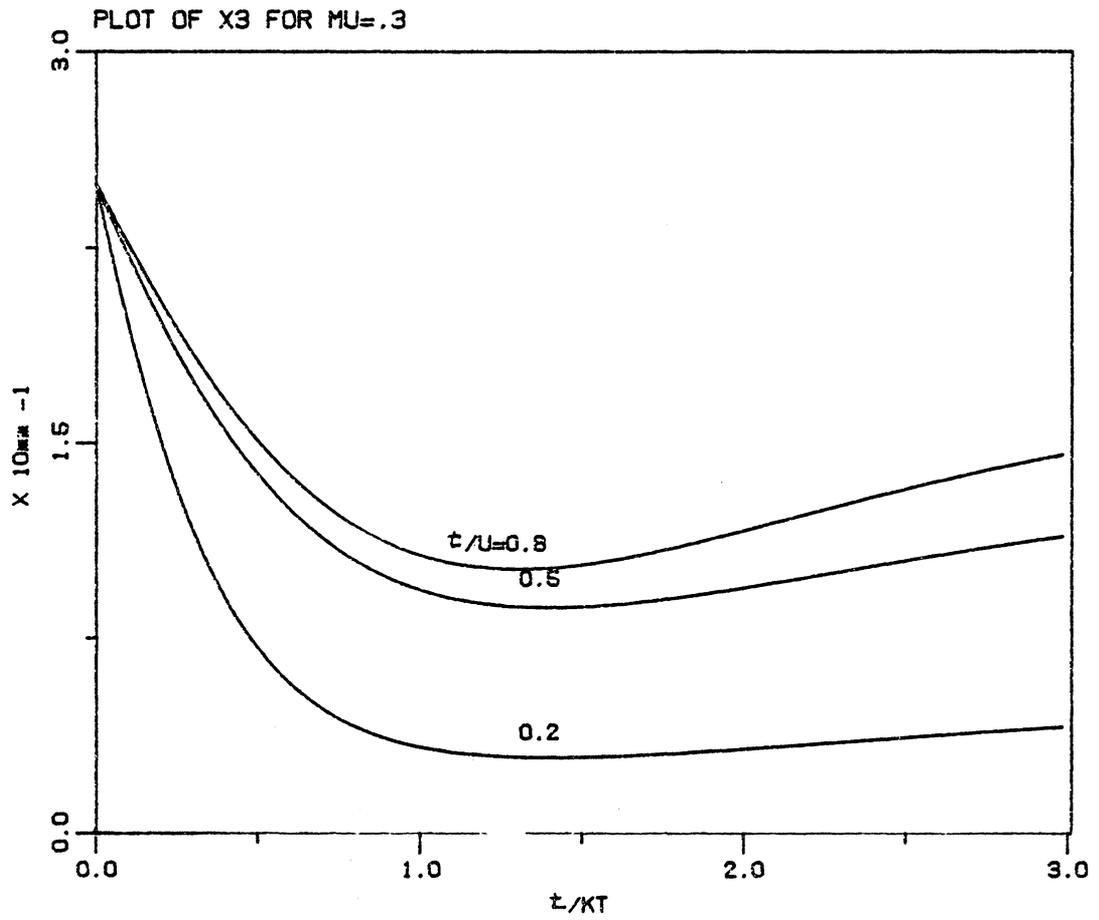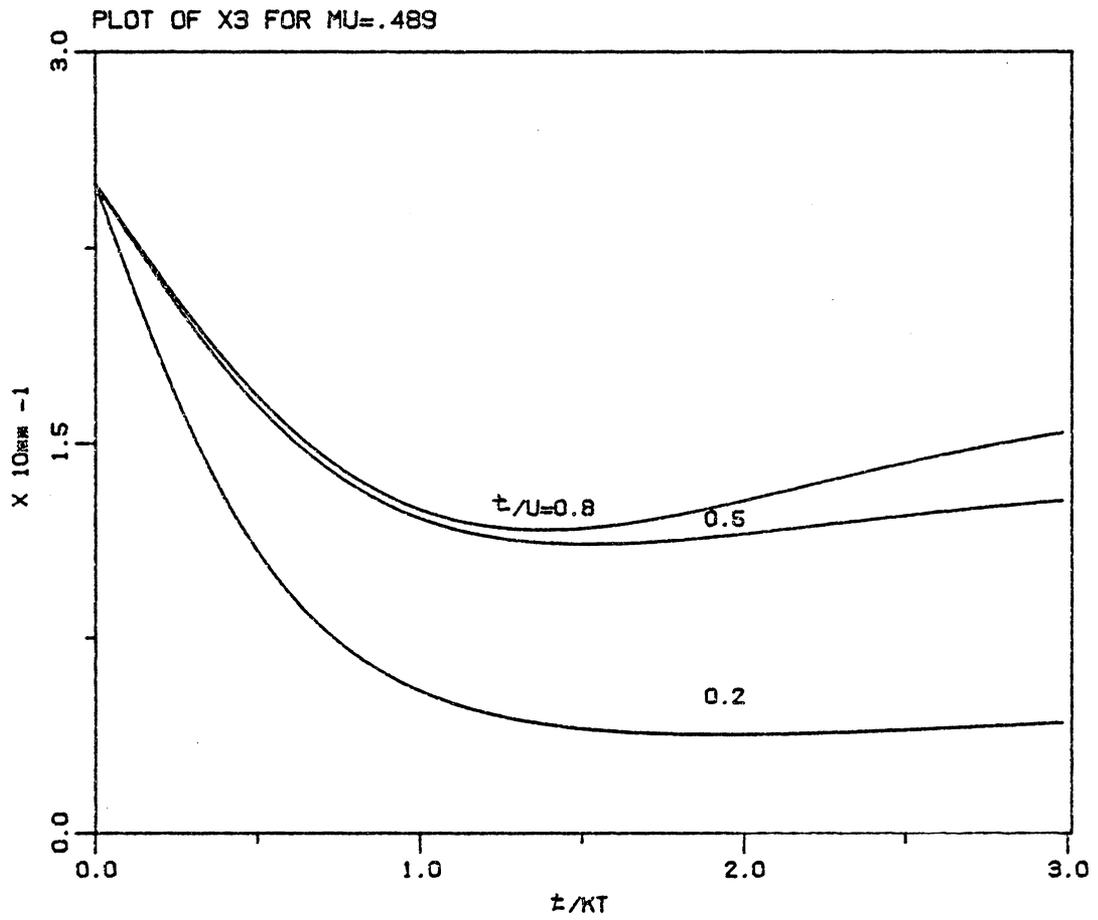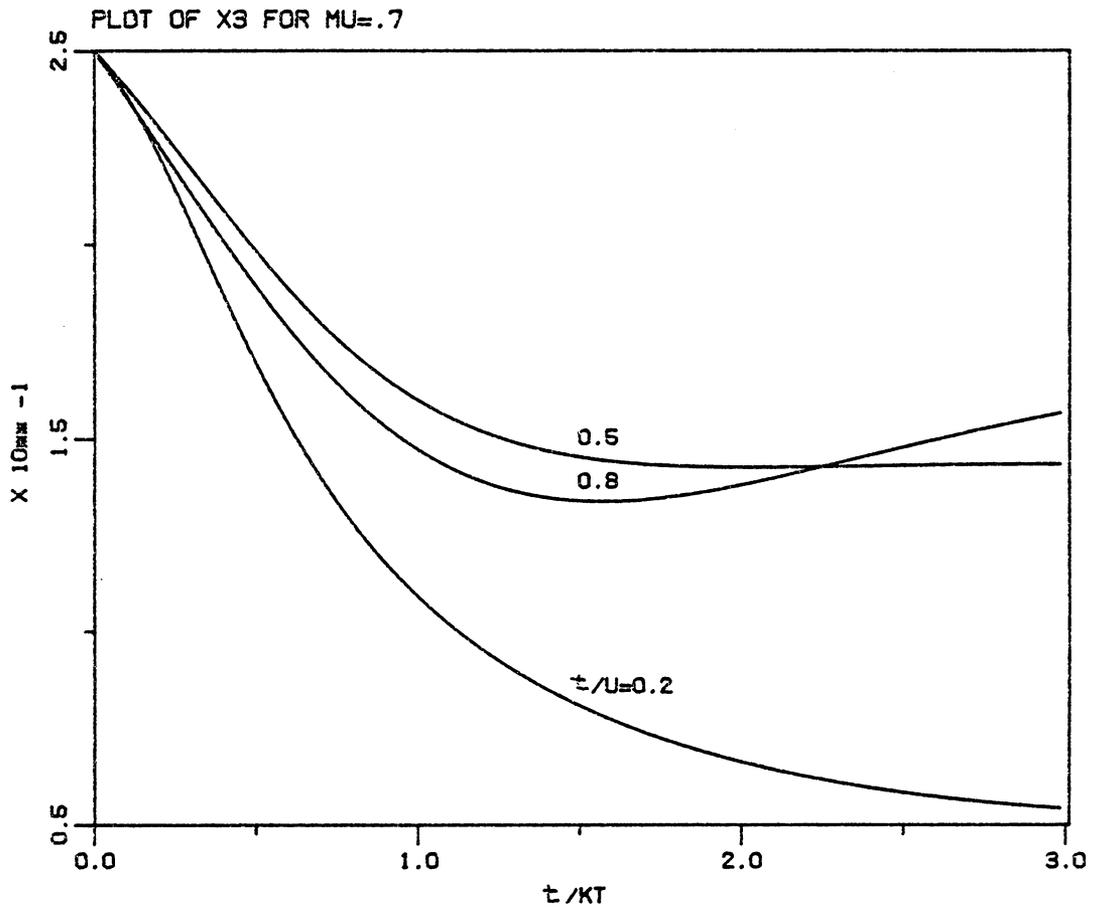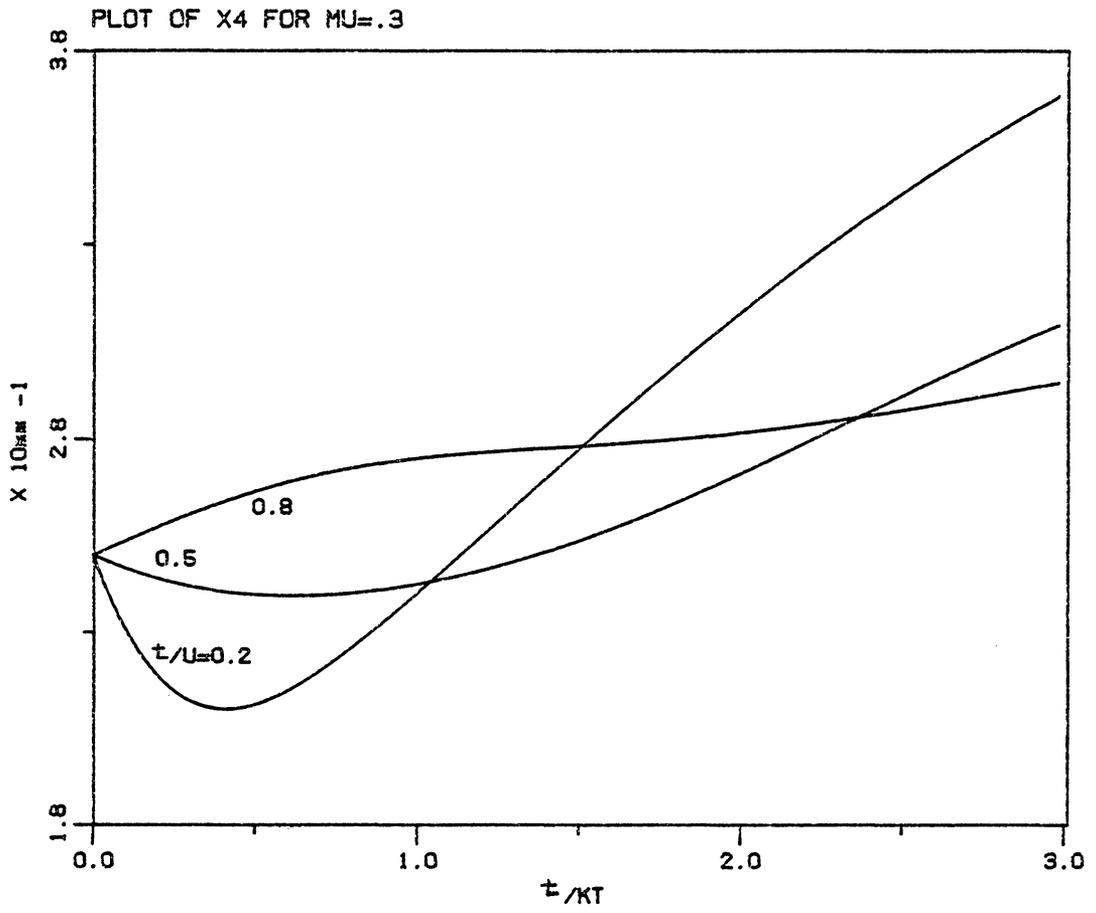
FIGURE 8.

FIGURE 9.

FIGURE 10.
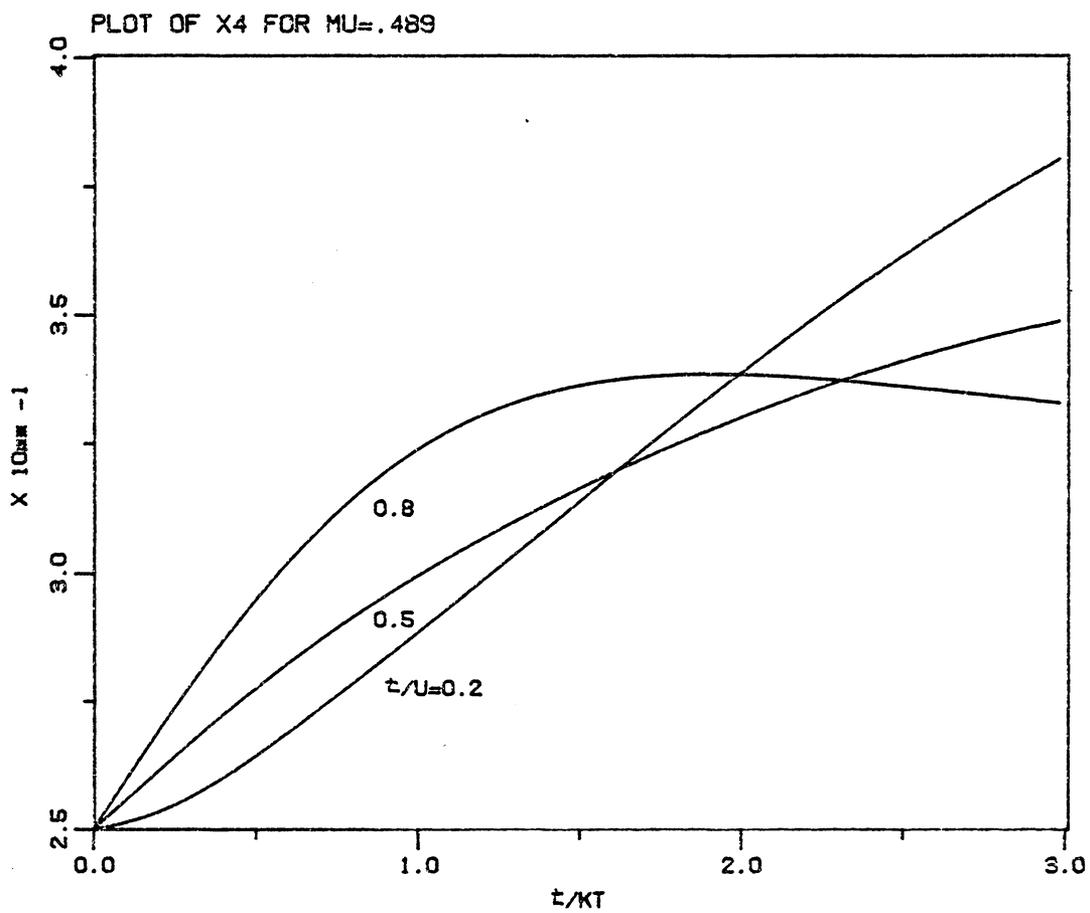
FIGURE 11.
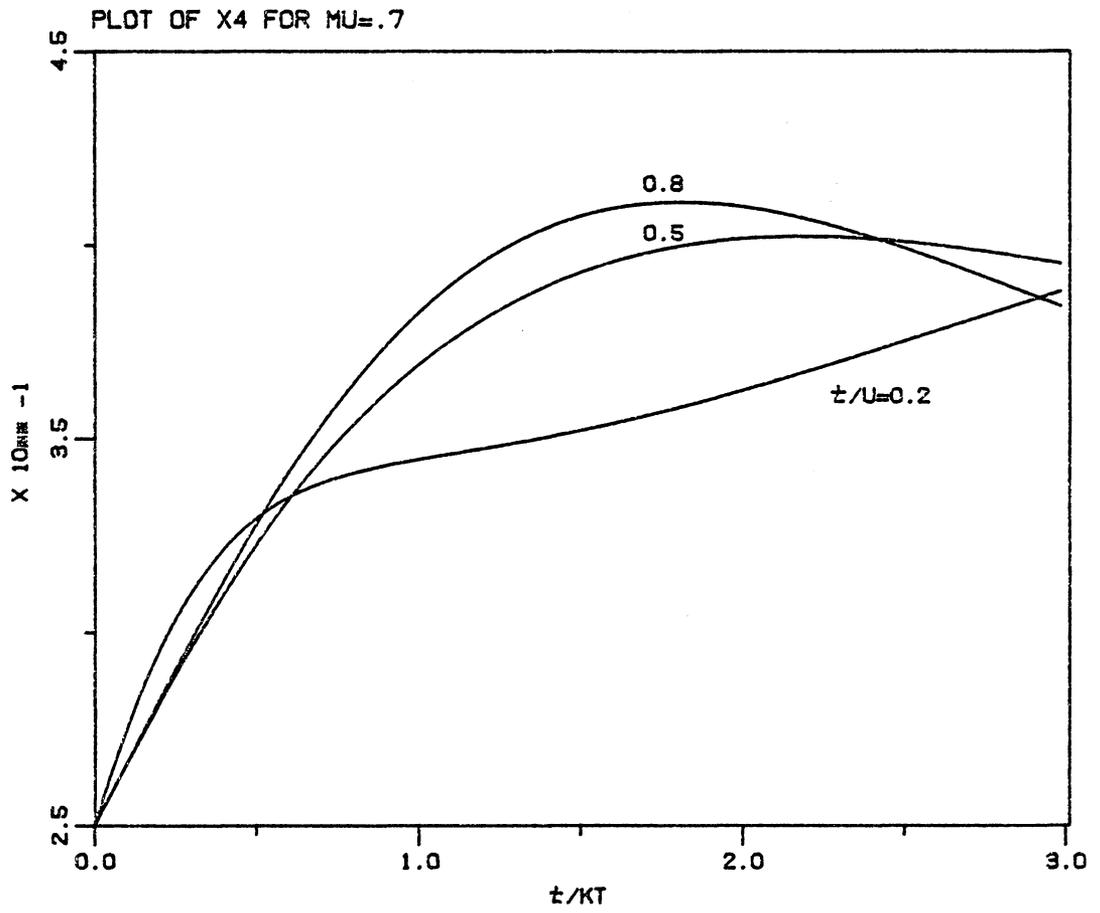
FIGURE 12.

FIGURE 13.

FIGURE 14.

PLOT OF X5 FOR MU=.7

$t/U=0.8$
0.5
0.2

X 10$\times$ −1

$t_{/KT}$
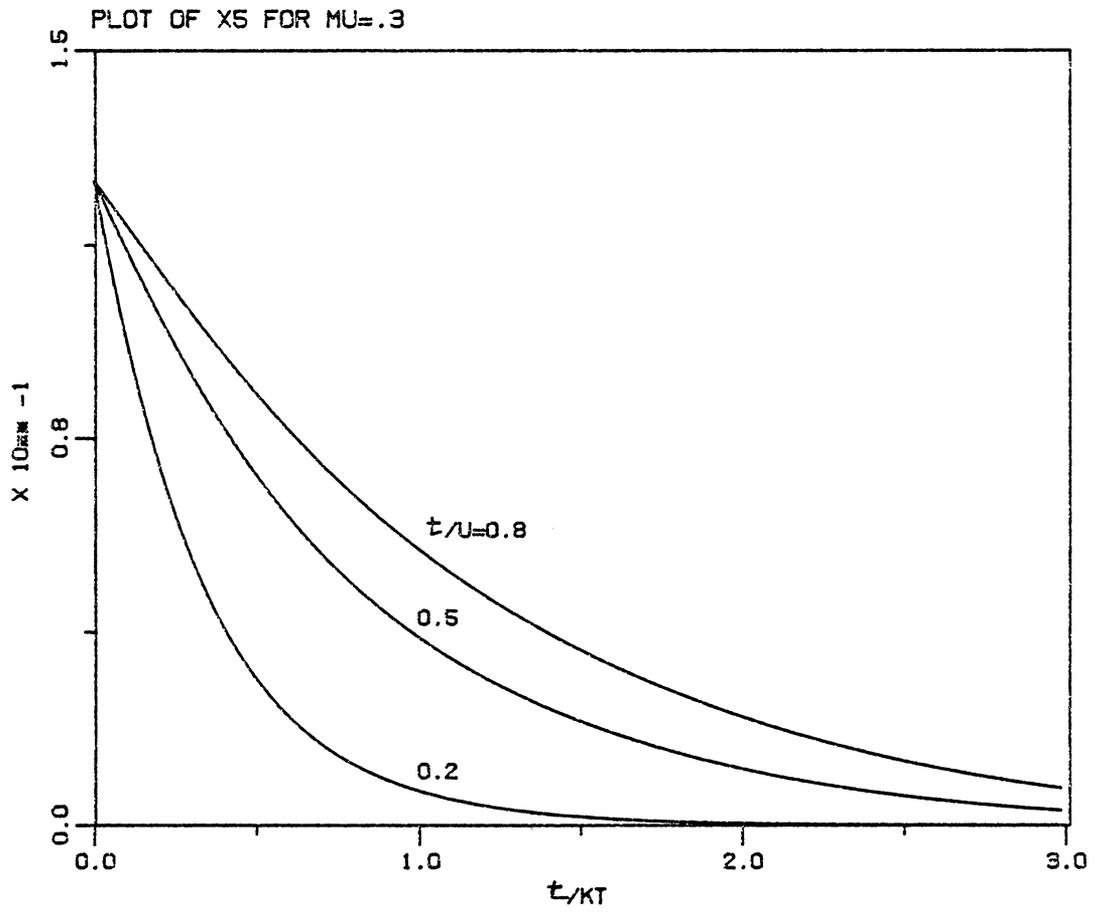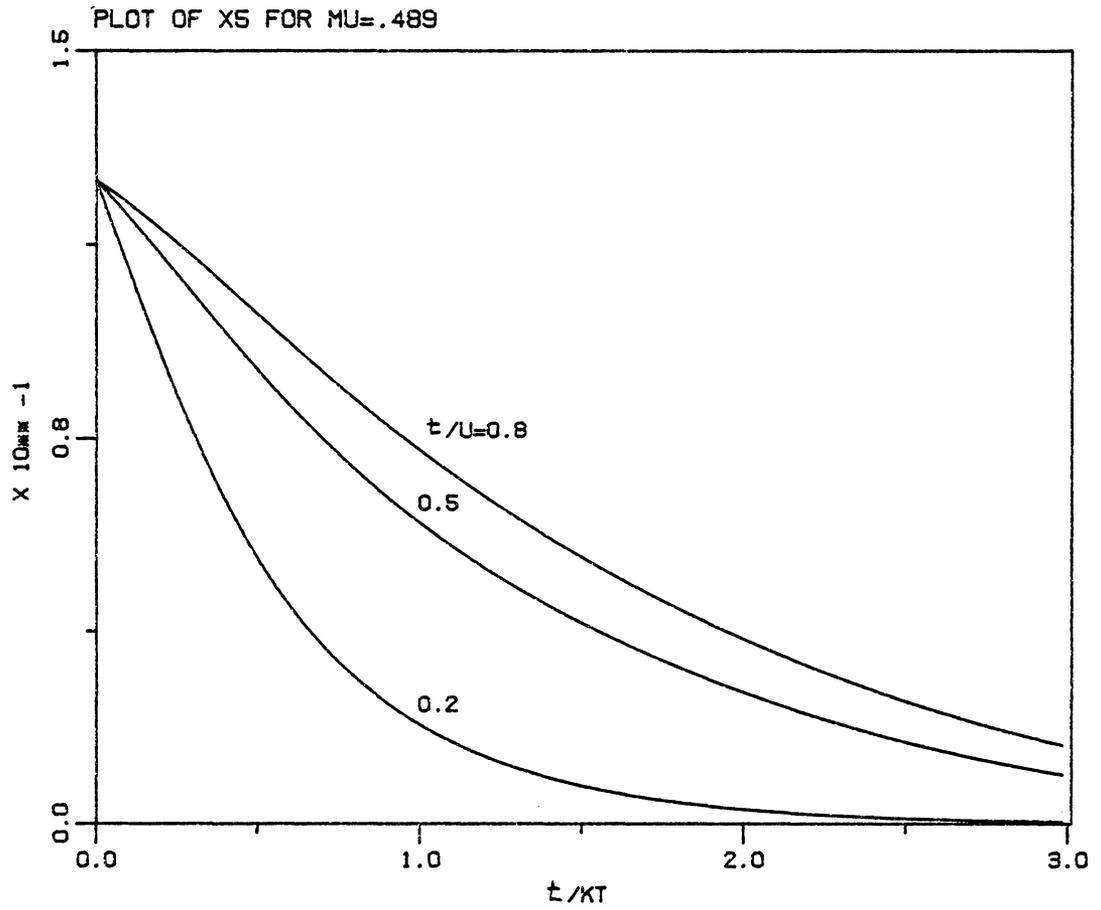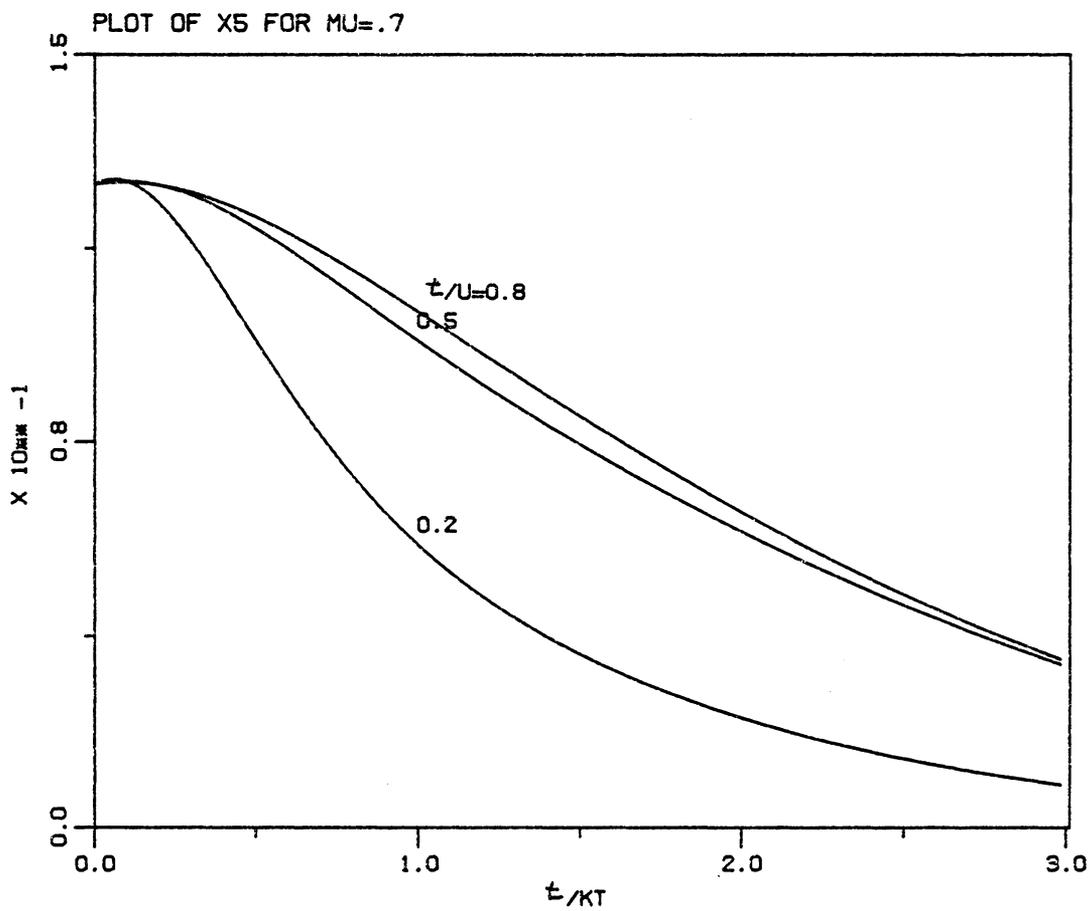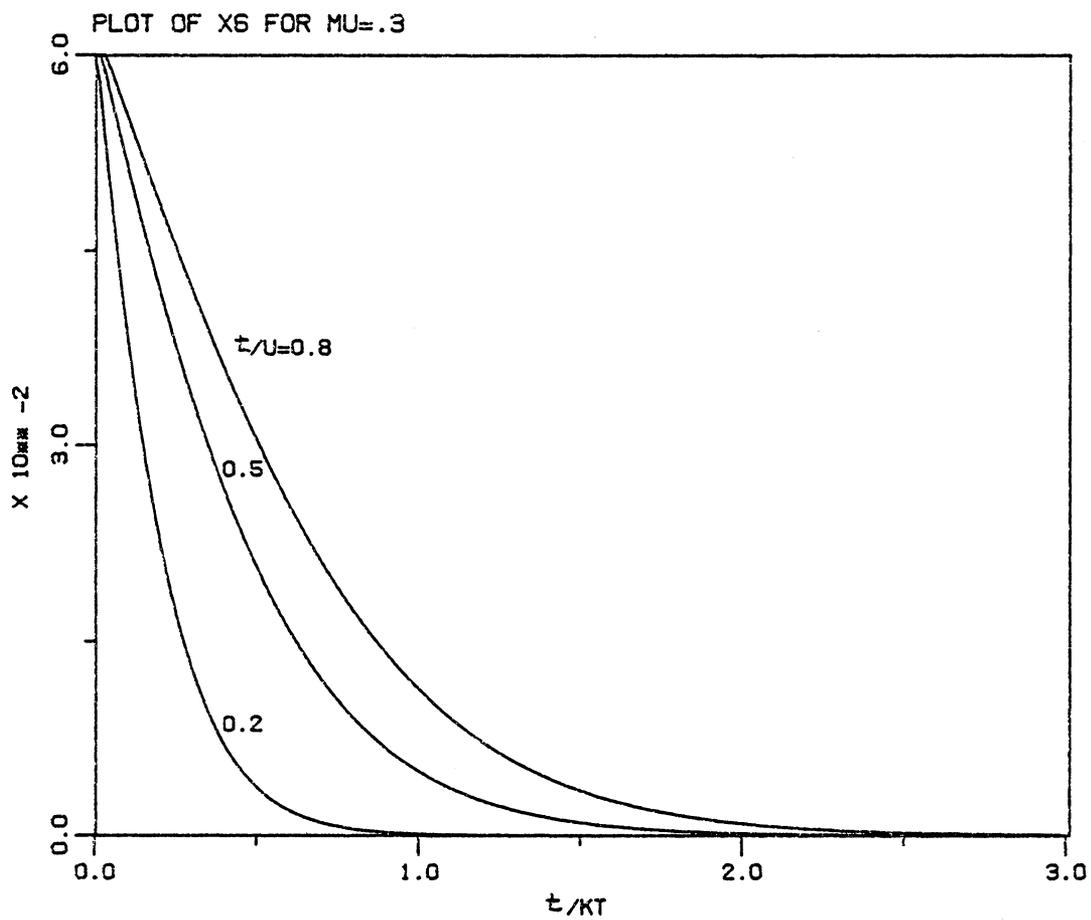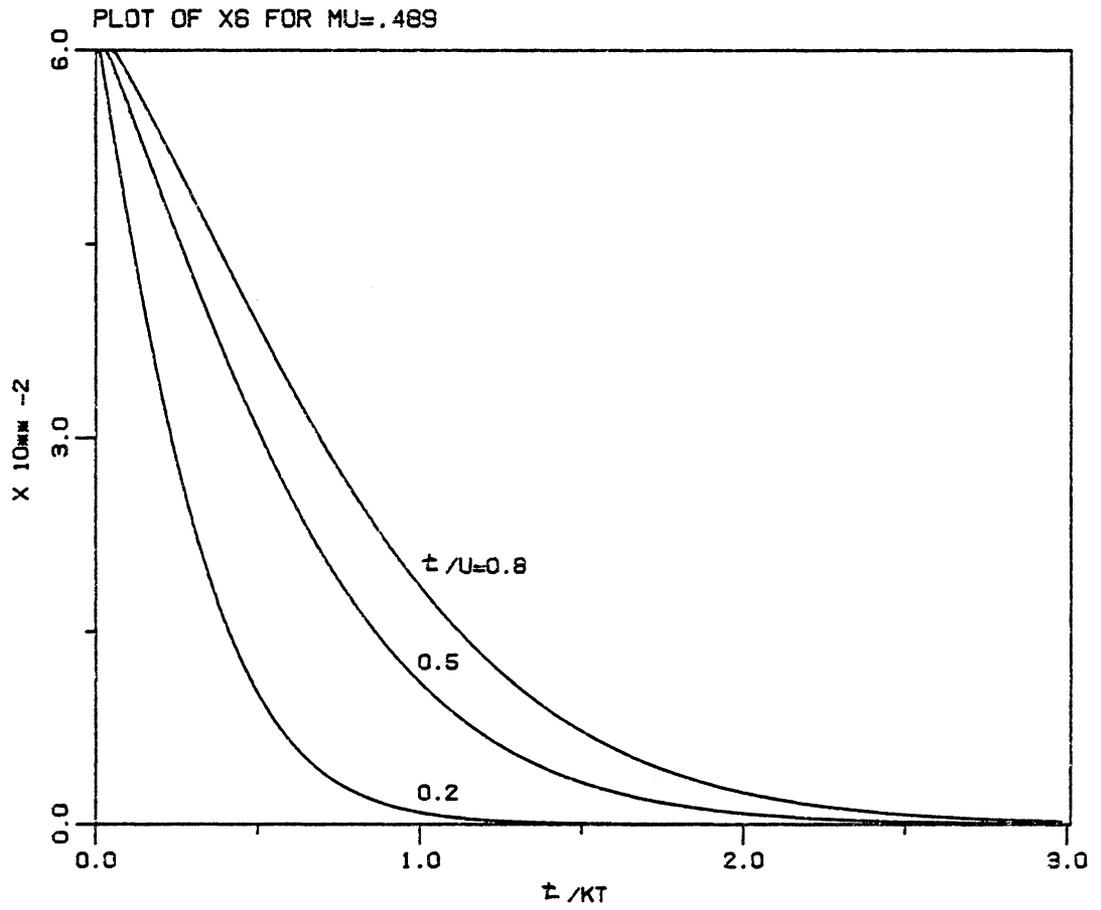
FIGURE 15.

FIGURE 16.

FIGURE 17.

FIGURE 18.

FIGURE 19.

PLOT OF X7 FOR MU=.489

FIGURE 20.

PLOT OF X7 FOR MU=.7

FIGURE 21.

FIGURE 22.

PLOT OF X8 FOR MU=.489
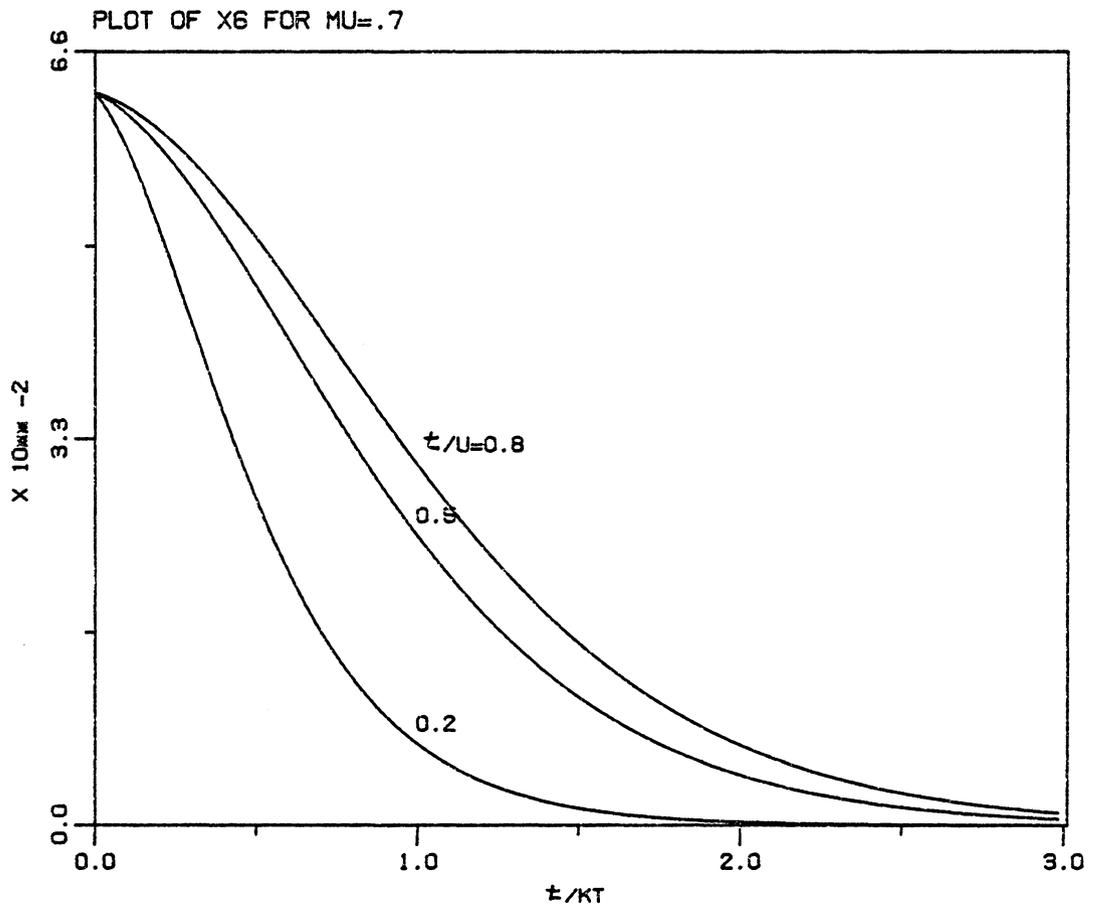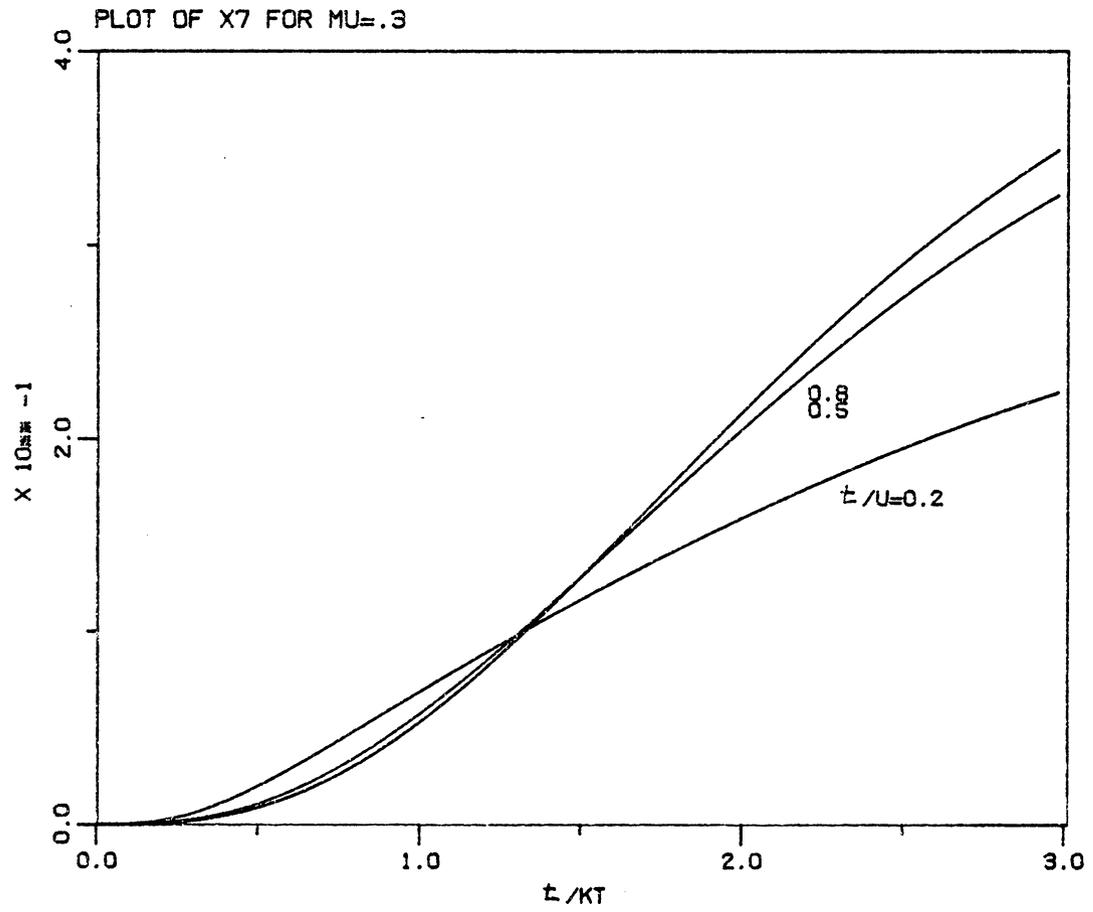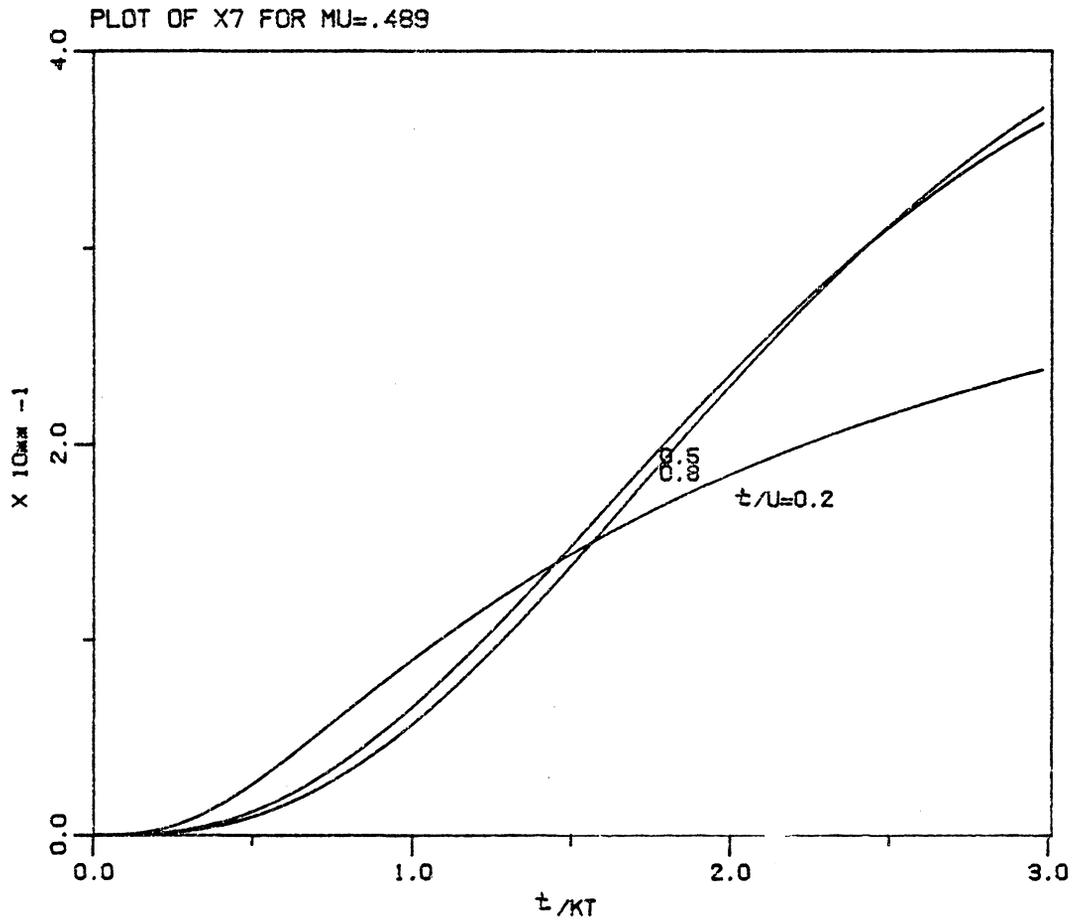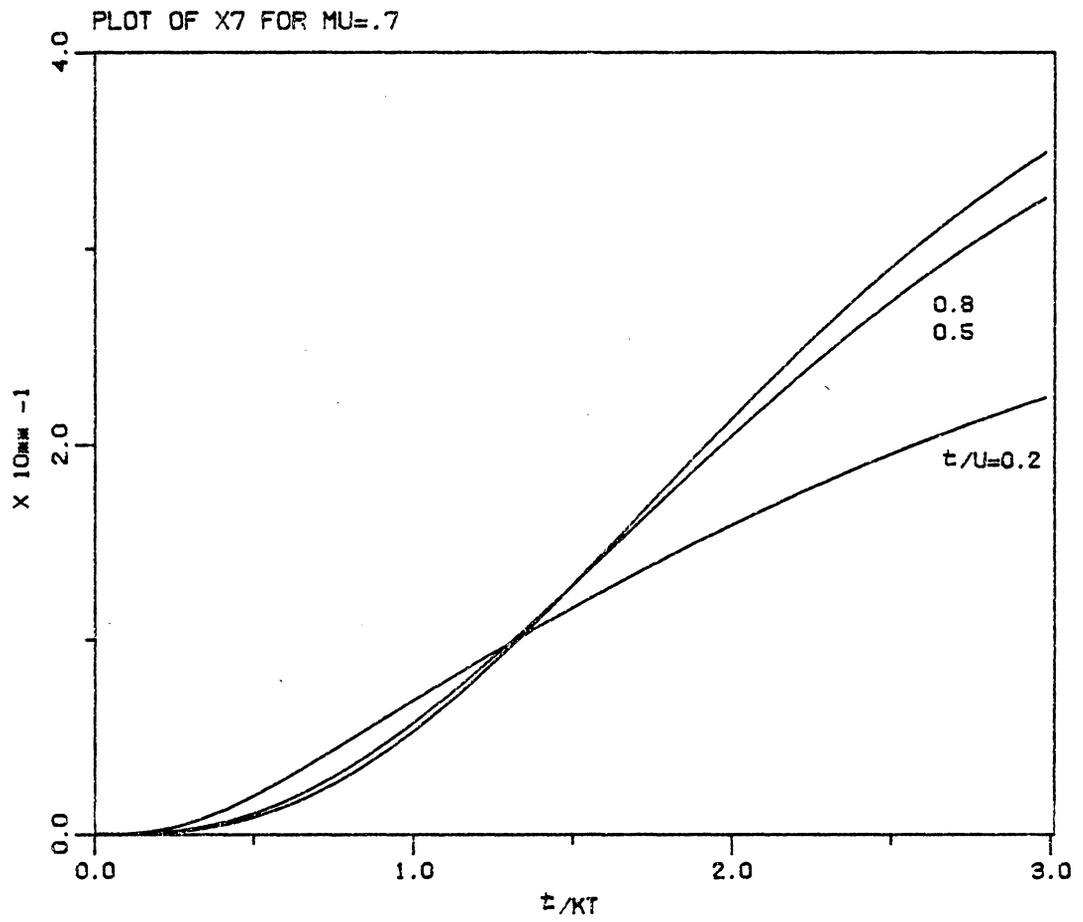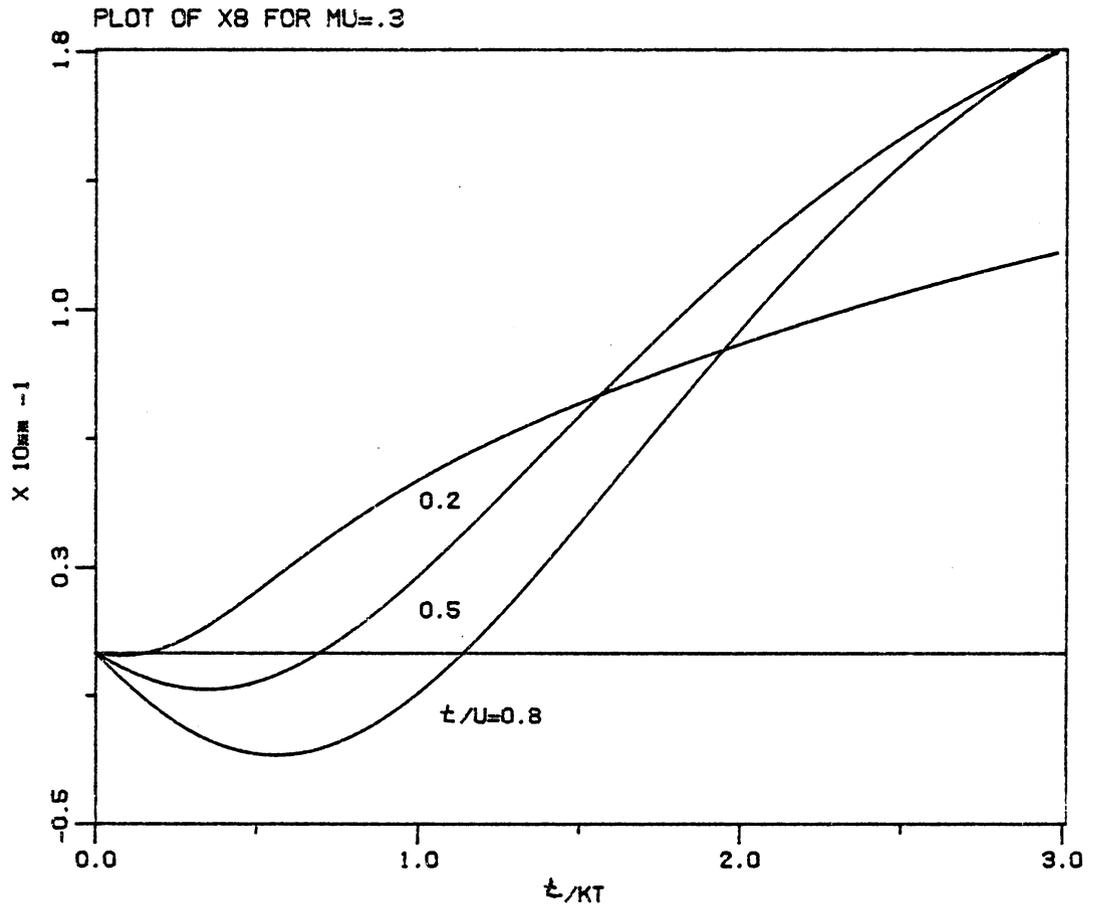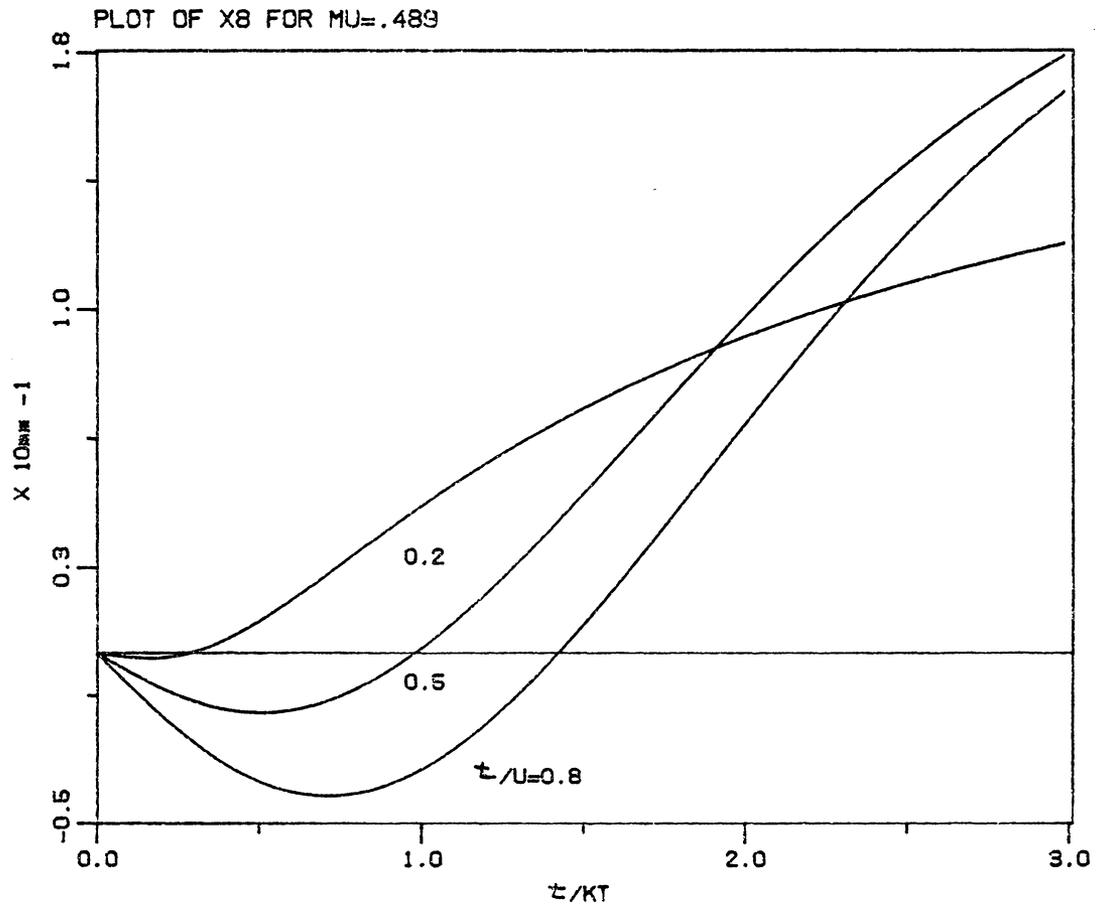
FIGURE 23.

FIGURE 24.

PLOT OF X9 FOR MU=.3
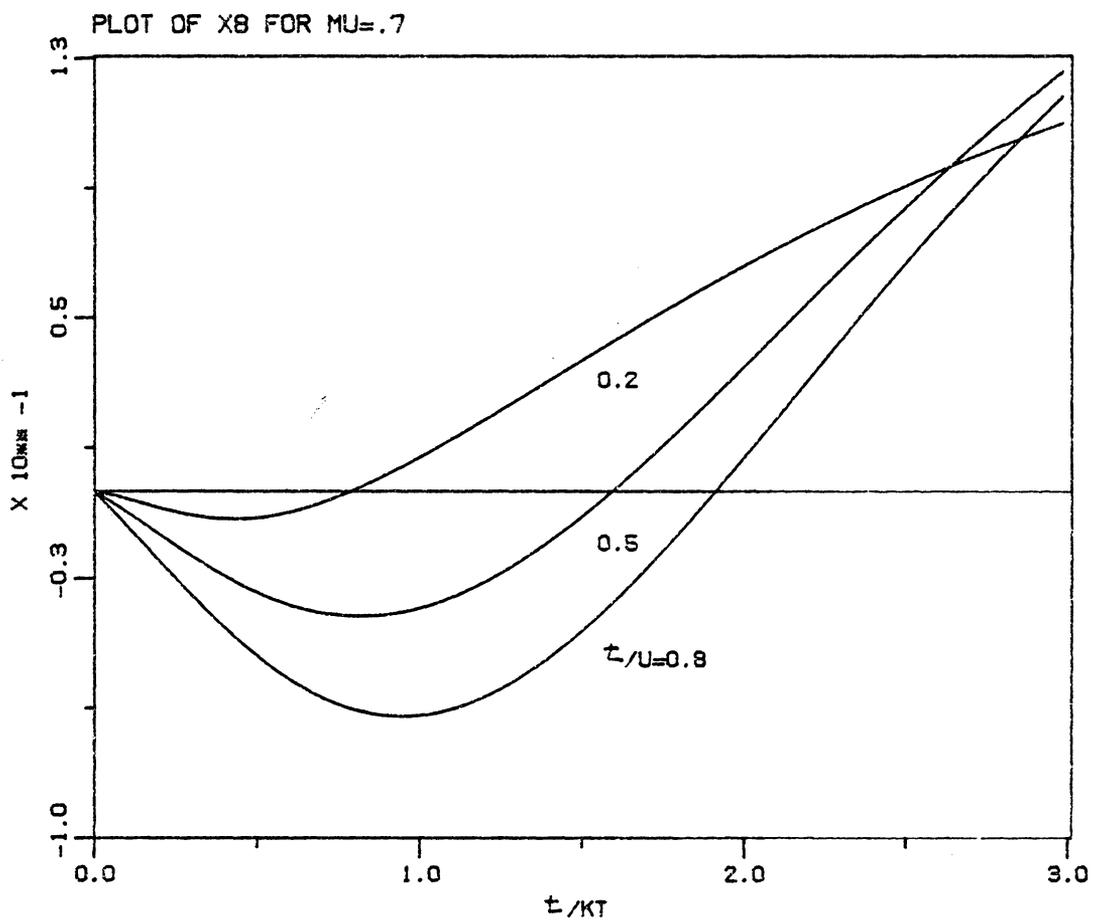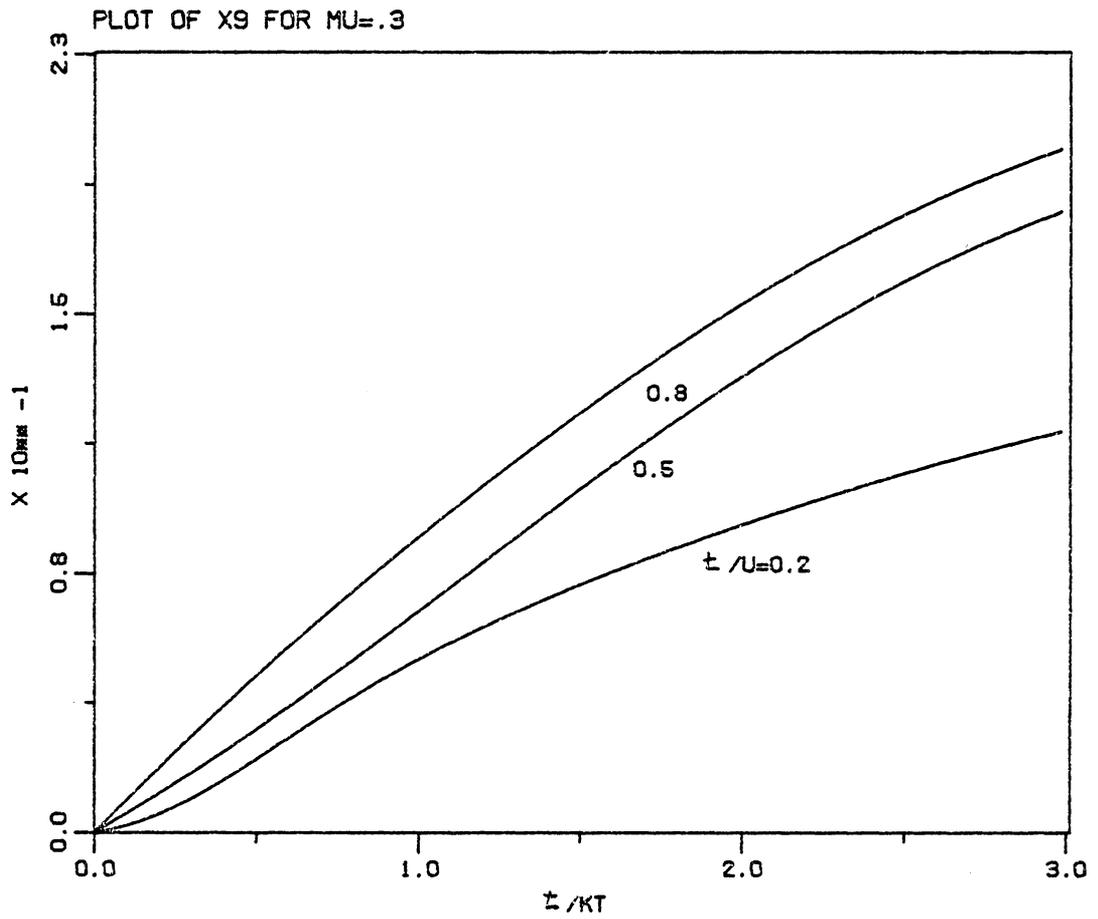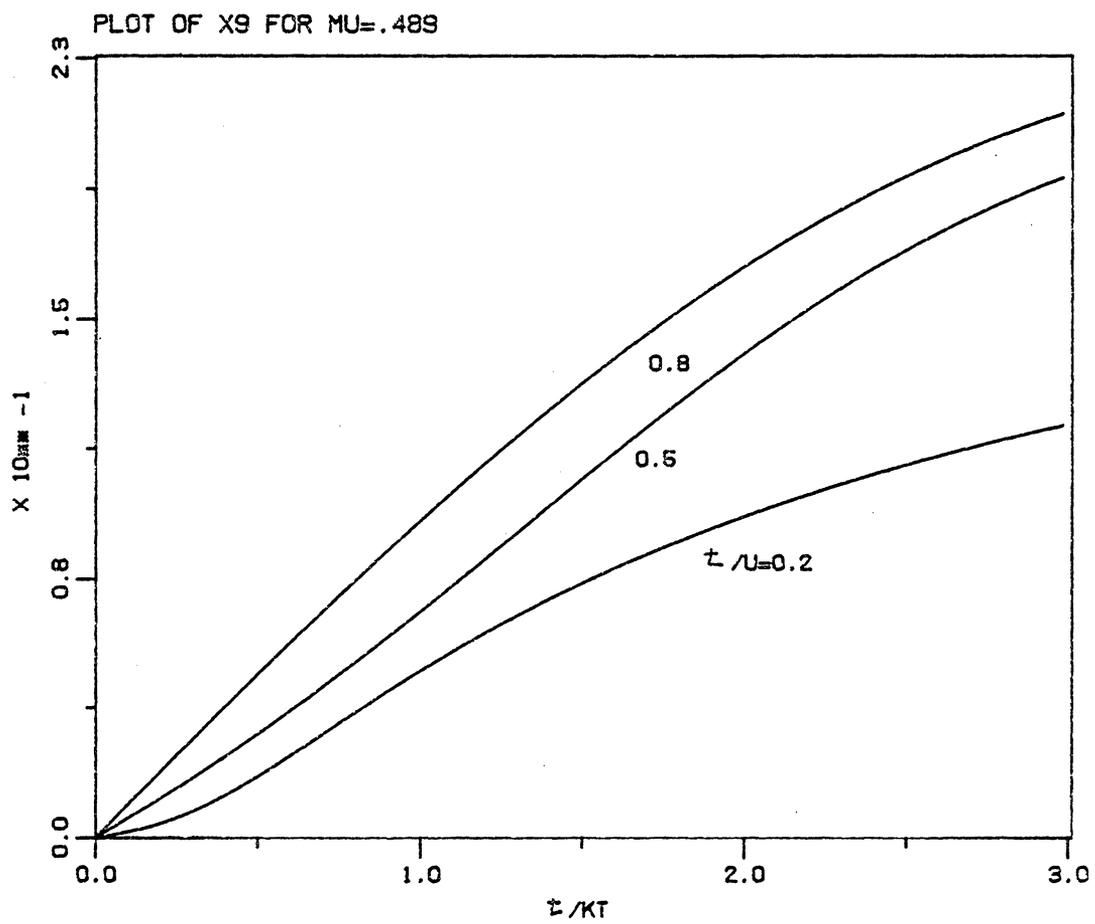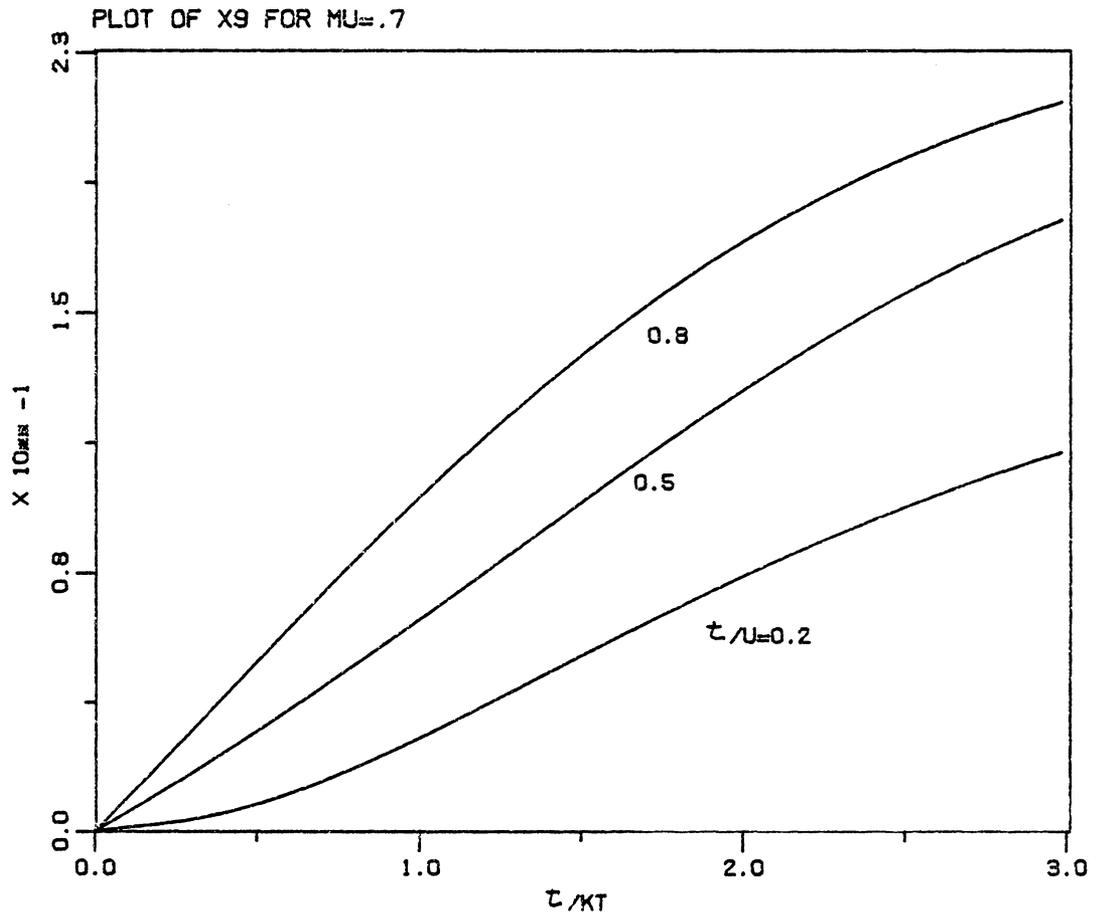
FIGURE 25.

FIGURE 26.

FIGURE 27.

FIGURE 28.

FIGURE 29.

PLOT OF X10 FOR MU=.7

X 10mm -2

t/U=0.2

0.5

0.8

t/KT
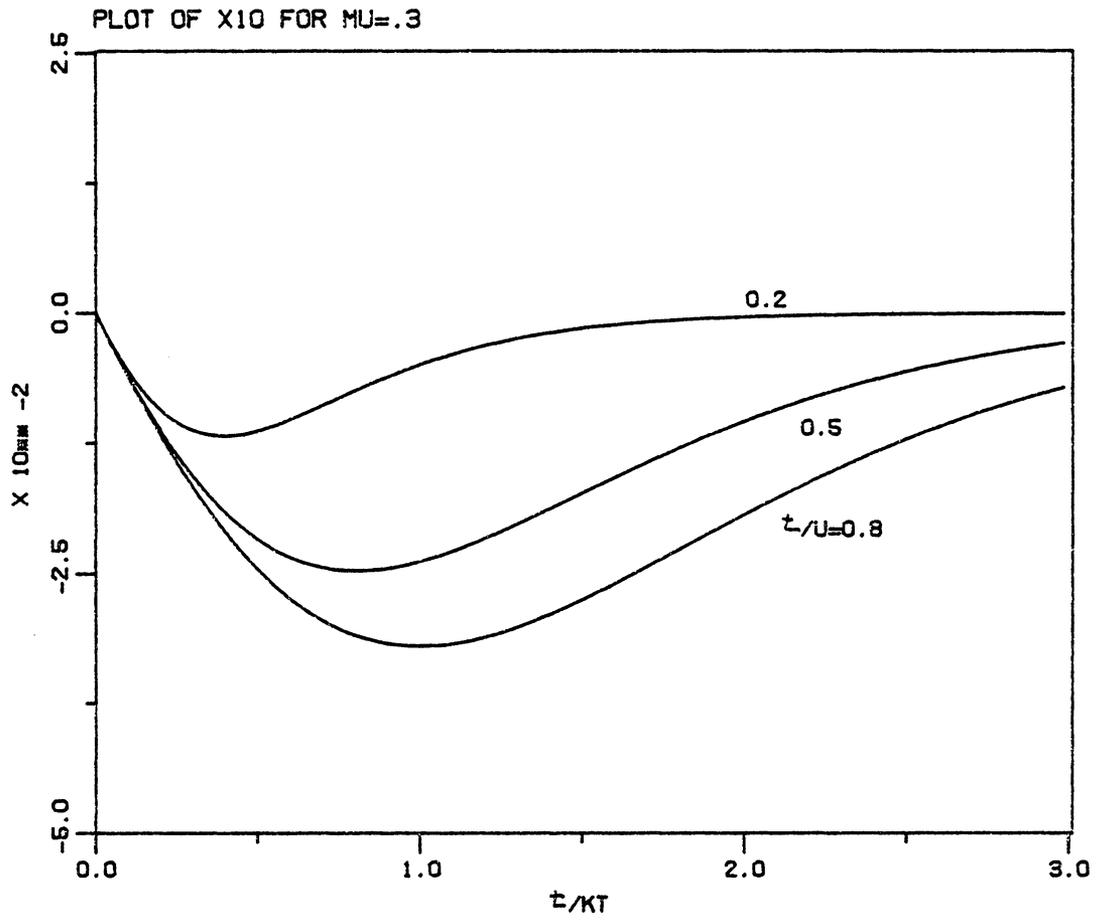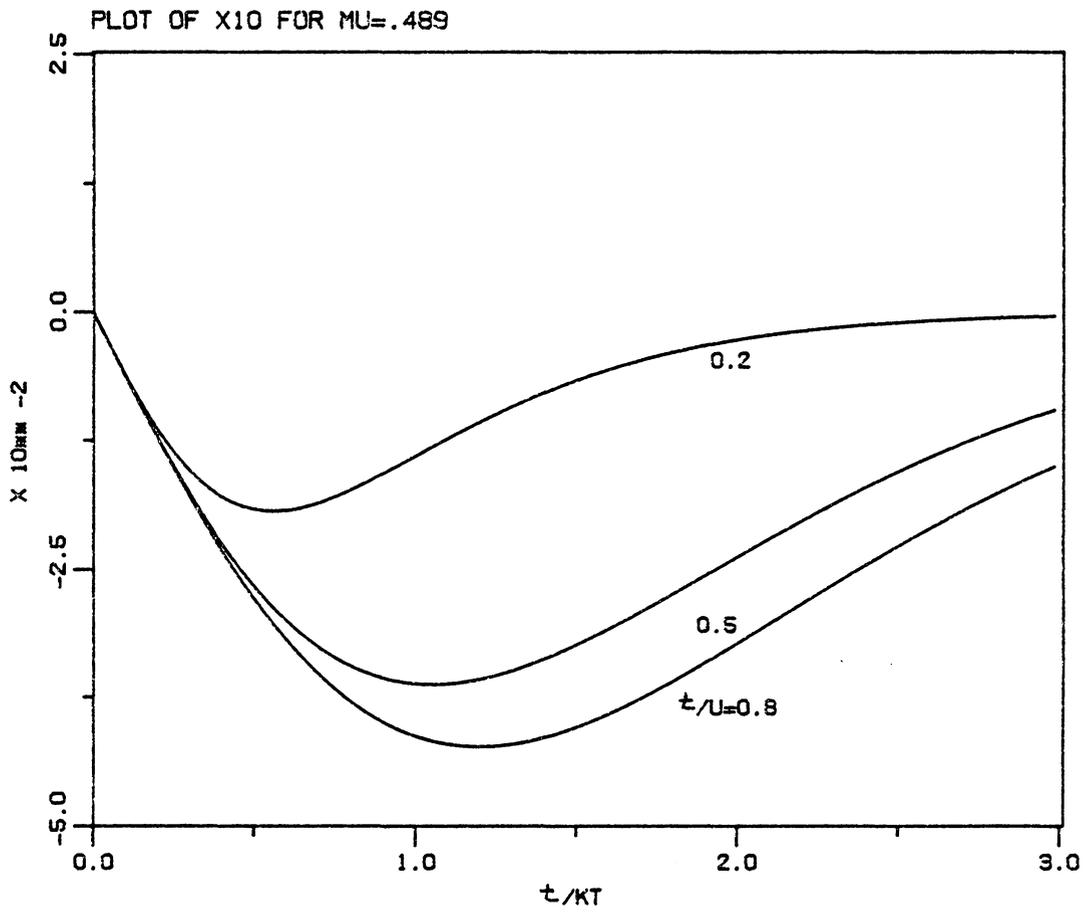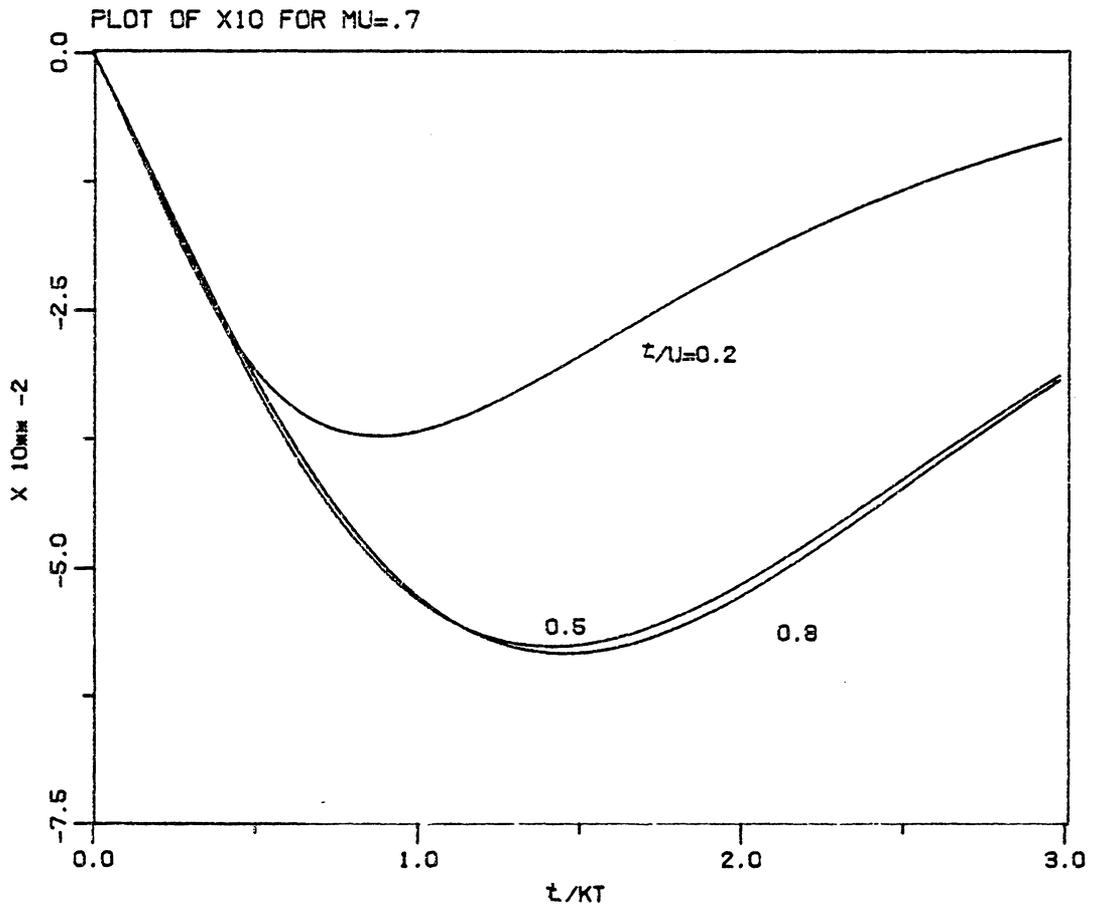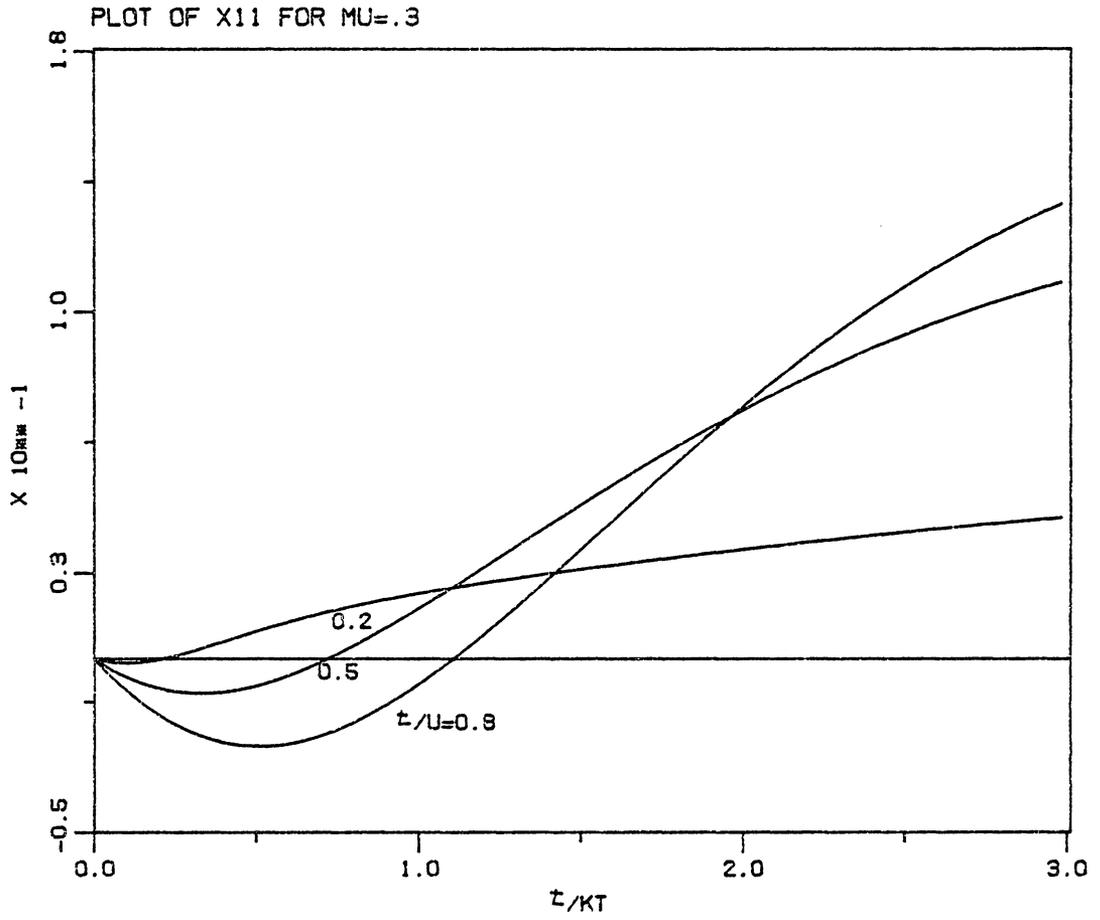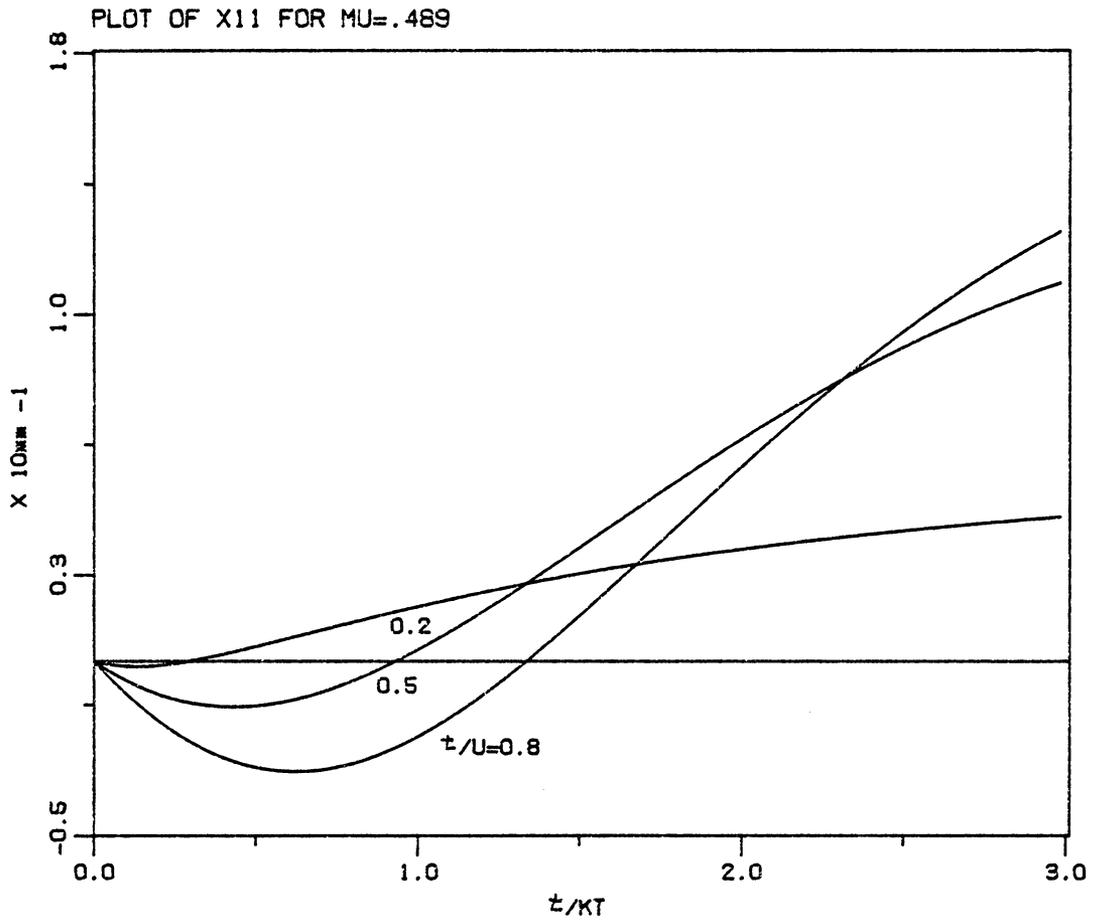
FIGURE 30.

FIGURE 31.

FIGURE 32.
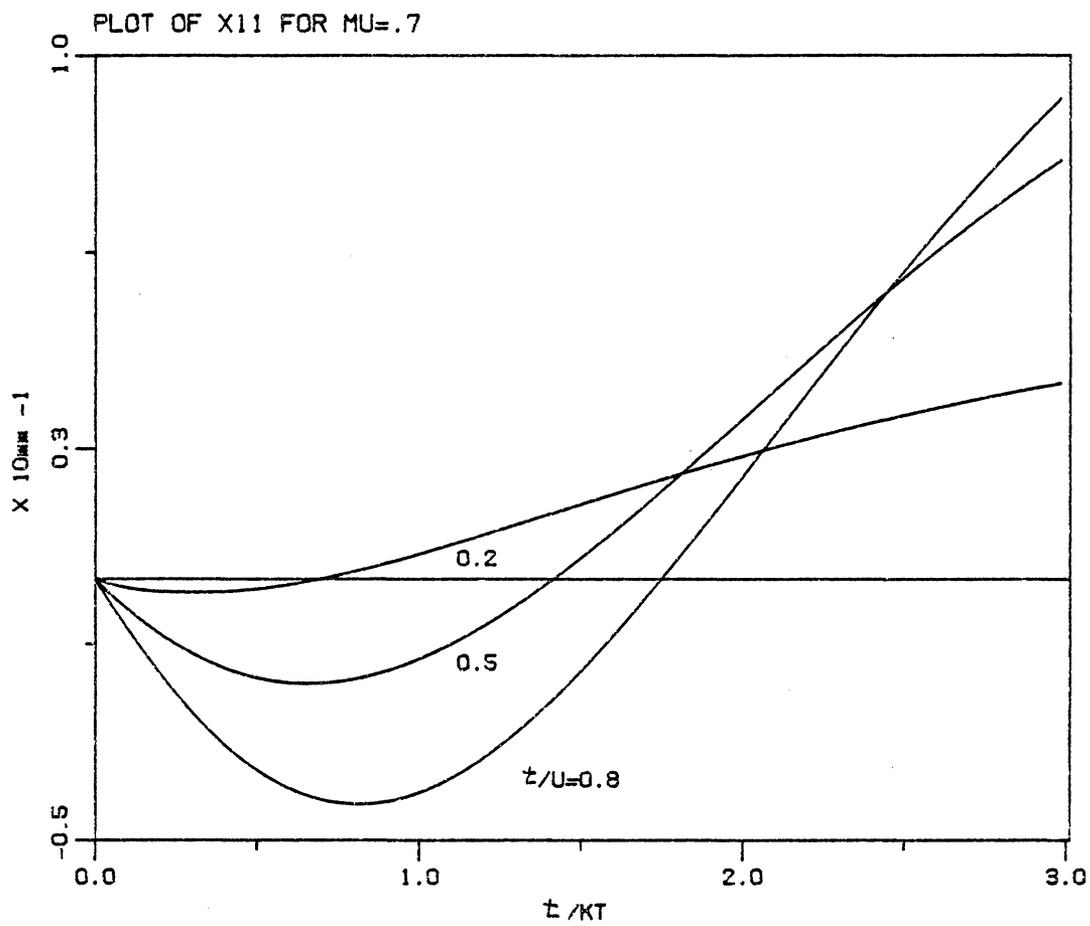
FIGURE 33.
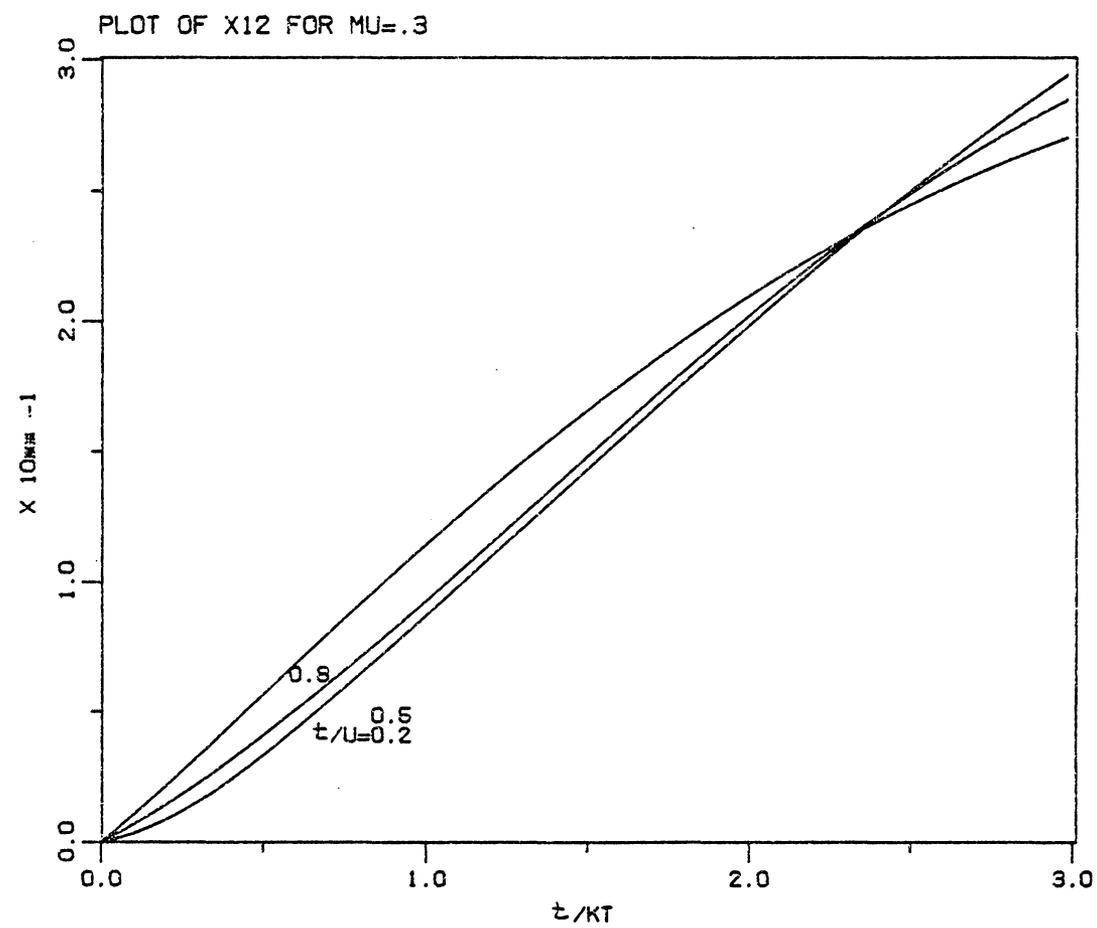
FIGURE 34.
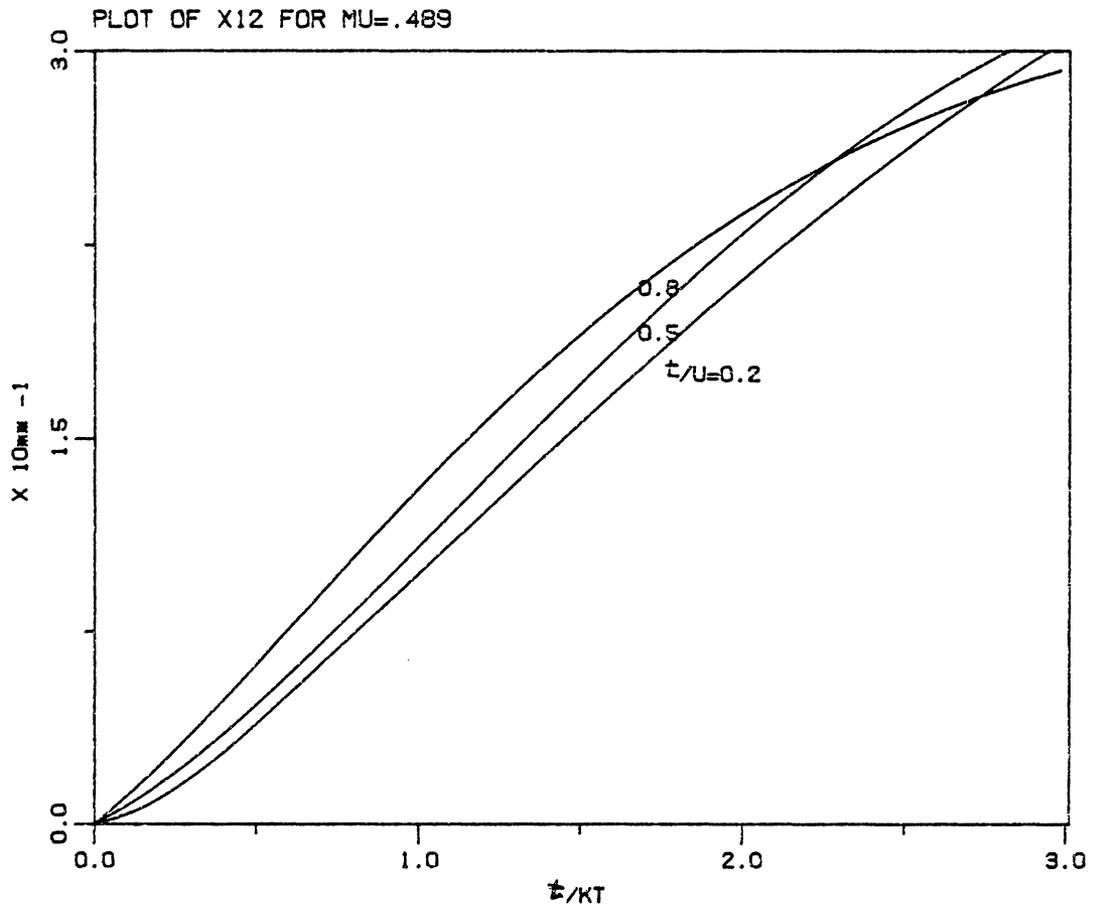
FIGURE 35.
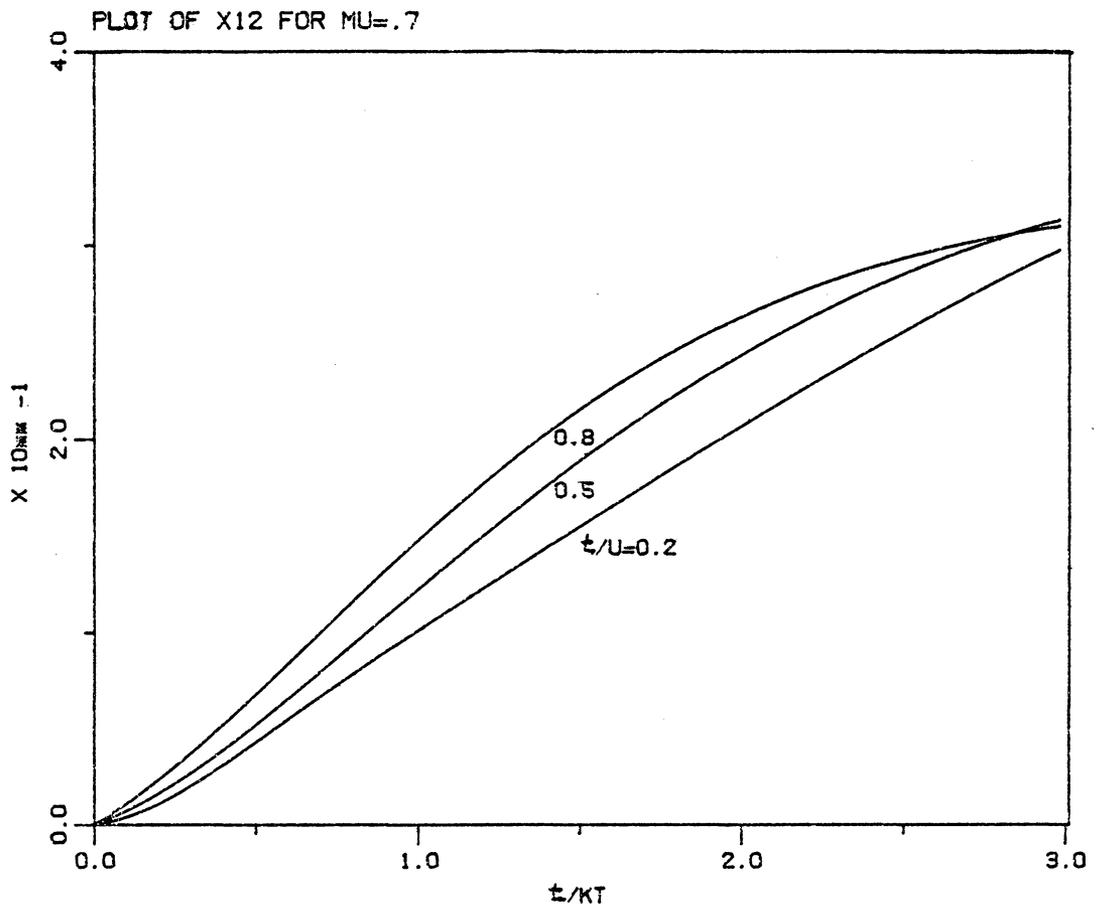
FIGURE 36.

calculations on the Hubbard model have been for the half-filled band where the chemical potential has the value $\mu = \varepsilon + U/2$, i.e. μ is independent of temperature.[43] In general the chemical potential is a complicated function of the temperature. The Judd operator formalism has provided us with a calculational scheme whereby each of the twelve correlation functions may be investigated as a function of chemical potential. Figure 1 displays the low temperature behavior for X1 which is expected. As the chemical potential increases in value X1 should also increase. For a small enough value of T a certain amount of structure begins to reveal itself. Each of the four horizontal planes correspond respectively (in the direction of increasing chemical potential) to the dimer undergoing a change in particle number of $0 \to 1$, $1 \to 2$, $2 \to 3$, and $3 \to 4$. The value of the chemical potential at which each of these transitions occurs agrees with the zero-temperature analysis of the partition function.

The correlation functions X2, X3, X5, and X6 take on values generally less than their high-temperature limits as the temperature decreases, while X4 generally increases from its high temperature limit regardless of the value of the chemical potential. These results agree with calculations which were done on the half-filled band.[44, 45, 46] It is well known that the ground state of the half-filled band is anti-ferromagnetic.[47] This fact is supported by Figure 11 which shows the correlation function $X4 = \langle n_{1\uparrow} n_{2\downarrow} \rangle$ generally increasing with decreasing temperature for the near-half-filled band. The interesting data, however, is provided by Figures 10 and 12. Here X4 is plotted for values of the chemical potential which describe systems with non-half-filled bands. To make any predictions on the possible anti-ferromagnetic behavior of X4 for very low values of T

for a non-half-filled band would, at this point, encompass a considerable amount of guesswork on our part, but it is clear that qualitative departures from half-filled-band behavior are large. Work is currently being carried out on the Hubbard chain where it is hoped that the Judd operator formalism will help to clarify this point.

We now focus our attention on the remaining correlation functions X7, X8, X9, X10, X11 and X12. Each of these correlation functions is comprised of some combination of the fermion single-particle operators c and $c^{\dagger}$ with n's. Analysis of these functions becomes quite involved as one varies t, μ, and T. However, a few comments concerning particle-hole symmetry can be made. Recall that for all of our calculations we have chosen $\epsilon = 0$ and U = 1.0 eV. Hence, as was mentioned previously (see reference 12) the value of the chemical potential for the half-filled band is given (independent of temperature) by $\mu = \epsilon + U/2 = 0.5$ eV. Note that all of our plots involve values of the chemical potential either near the half-filled value, at 0.489, or for values symmetric about 0.5 eV, i.e. 0.3 and 0.7 eV. Naively one might expect some sort of symmetry about $\mu = 0.5$ eV to be present, allowing for particle-hole symmetry. A brief glimpse of the accompanying figures reveals that in general there is no such symmetry. However, we do note a definite symmetry pattern about $\mu = 0.5$ eV for those plots involving either X1 or X7. In fact X1-0.5 is precisely anti-symmetric about $\mu = 0.5$ eV while X7 is symmetric. That this is required can be shown mathematically in a straightforward manner using particle-hole symmetry. The point to be made is that both X1 and X7 are single-particle correlation

functions, so the symmetry involved with respect to the chemical potential

is to be expected since the chemical potential is manifestly a single-

particle quantity. Similarly, the lack of any sort of symmetry about the

half-filled band value of μ for the ten remaining correlation functions

is also to be expected since all of these are two-and three-particle

correlation functions. We would like to point out also that there exists

certain discrepancies between our work and that of Chen[45] and Chen and

Huang.[46] The most pronounced differences occur for the correlation func-

tions X8 and X10 for values of μ near the half-filled band value.

Considerations of appropriate high-temperature limits (in the context of

our analysis) support the results presented in Figures 23 and 29.

For approximately the past quarter of a century the field of many-

body physics has been monopolized by certain standard methods of calculation.

In these pages we have laid down principal elements of the foundations of

a new method of calculation while also applying it to the Hubbard dimer.

The hope is that the Judd operator formalism will become a part of the

standard repertoire of the many-body theorist. The full calculational

potential of the method is as yet untested although current investigation

is underway on the problems of the Hubbard chain, the periodic Anderson

model, and other models for mixed-valence compounds. The utility of a

method involving many-particle stepping operators seems manifest for

mixed-valence compounds where d and f electron numbers are fluctuating.

However, until applications of the method are carried out on non-trivial

models such as those just mentioned, the Judd operator formalism will

remain an attractive but unproven alternative calculational scheme in many-body physics.

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We list the complete set of stepping operators and orthogonal projection operators for the Hubbard dimer.

Single-particle operators:

$$\phi_9 = c_{1\uparrow}^\dagger c_{1\downarrow}^\dagger c_{2\uparrow}^\dagger I_\Theta c_{2\downarrow} c_{2\uparrow} c_{1\downarrow} c_{1\uparrow} = -n_{2\uparrow} n_{1\downarrow} n_{1\uparrow} c_{2\downarrow}$$

$$\phi_{9p} = c_{1\uparrow}^\dagger c_{2\uparrow}^\dagger c_{2\downarrow}^\dagger I_\Theta c_{2\downarrow} c_{2\uparrow} c_{1\downarrow} c_{1\uparrow} = -n_{1\uparrow} n_{2\downarrow} n_{2\uparrow} c_{1\downarrow}$$

$$\phi_{10} = c_{1\uparrow}^\dagger c_{2\uparrow}^\dagger I_\Theta c_{2\uparrow} c_{1\downarrow} c_{1\uparrow} = -n_{2\uparrow} n_{1\uparrow} (1-n_{2\downarrow}) c_{1\downarrow}$$

$$\phi_{10p} = c_{1\uparrow}^\dagger c_{2\uparrow}^\dagger I_\Theta c_{2\downarrow} c_{2\uparrow} c_{1\uparrow} = -n_{2\uparrow} n_{1\uparrow} (1-n_{1\downarrow}) c_{2\downarrow}$$

$$\phi_{11} = c_{1\uparrow}^\dagger c_{1\downarrow}^\dagger I_\Theta c_{2\downarrow} c_{1\downarrow} c_{1\uparrow} = n_{1\downarrow} n_{1\uparrow} (1-n_{2\uparrow}) c_{2\downarrow}$$

$$\phi_{11p} = c_{2\uparrow}^\dagger c_{2\downarrow}^\dagger I_\Theta c_{2\downarrow} c_{2\uparrow} c_{1\downarrow} = n_{2\downarrow} n_{2\uparrow} (1-n_{1\uparrow}) c_{1\downarrow}$$

$$\phi_{12} = c_{1\uparrow}^\dagger c_{2\downarrow}^\dagger I_\Theta c_{2\downarrow} c_{1\downarrow} c_{1\uparrow} = -n_{2\downarrow} n_{1\uparrow} (1-n_{2\uparrow}) c_{1\downarrow}$$

$$\phi_{12p} = -c_{1\downarrow}^\dagger c_{2\uparrow}^\dagger I_\Theta c_{2\downarrow} c_{2\uparrow} c_{1\downarrow} = -n_{1\downarrow} n_{2\uparrow} (1-n_{1\uparrow}) c_{2\downarrow}$$

$$\phi_{13} = c_{1\uparrow}^\dagger I_\Theta c_{1\downarrow} c_{1\uparrow} = -n_{1\uparrow} (1-n_{2\uparrow})(1-n_{2\downarrow}) c_{1\downarrow}$$

$$\phi_{13p} = c_{2\uparrow}^\dagger I_\Theta c_{2\downarrow} c_{2\uparrow} = -n_{2\uparrow} (1-n_{1\uparrow})(1-n_{1\downarrow}) c_{2\downarrow}$$

$$\phi_{14} = c_{1\uparrow}^\dagger I_\Theta c_{2\downarrow} c_{1\uparrow} = -n_{1\uparrow} (1-n_{1\downarrow})(1-n_{2\uparrow}) c_{2\downarrow}$$

$$\phi_{14p} = -c_{2\uparrow}^\dagger I_\Theta c_{2\uparrow} c_{1\downarrow} = -n_{2\uparrow} (1-n_{2\downarrow})(1-n_{1\uparrow}) c_{1\downarrow}$$

$$\phi_{15} = c_{1\downarrow}^{\dagger} I_{\theta} c_{2\downarrow} c_{1\downarrow} = -n_{1\downarrow}(1-n_{1\uparrow})(1-n_{2\uparrow})c_{2\downarrow}$$

$$\phi_{15_p} = -c_{2\downarrow}^{\dagger} I_{\theta} c_{2\downarrow} c_{1\downarrow} = -n_{2\downarrow}(1-n_{2\uparrow})(1-n_{1\uparrow})c_{1\downarrow}$$

$$\phi_{16} = I_{\theta} c_{1\downarrow} = (1-n_{2\uparrow})(1-n_{2\downarrow})(1-n_{1\uparrow})c_{1\downarrow} .$$

$$\phi_{16_p} = I_{\theta} c_{2\downarrow} = (1-n_{1\uparrow})(1-n_{1\downarrow})(1-n_{2\uparrow})c_{2\downarrow}$$

$$\tilde{\phi}_{17} = c_{1\downarrow}^{\dagger} c_{2\downarrow}^{\dagger} I_{\theta} c_{2\uparrow} c_{1\downarrow} c_{1\uparrow} = n_{1\downarrow} c_{2\downarrow}^{\dagger} c_{2\uparrow} c_{1\uparrow}$$

$$\tilde{\phi}_{17_p} = -c_{1\downarrow}^{\dagger} c_{2\downarrow}^{\dagger} I_{\theta} c_{2\downarrow} c_{2\uparrow} c_{1\uparrow} = -n_{2\downarrow} c_{1\downarrow}^{\dagger} c_{2\uparrow} c_{1\uparrow}$$

$$\tilde{\phi}_{18} = c_{1\uparrow}^{\dagger} c_{2\uparrow}^{\dagger} I_{\theta} c_{2\downarrow} c_{1\downarrow} c_{1\uparrow} = -n_{1\uparrow} c_{2\uparrow}^{\dagger} c_{2\downarrow} c_{1\downarrow}$$

$$\tilde{\phi}_{18_p} = -c_{1\uparrow}^{\dagger} c_{2\uparrow}^{\dagger} I_{\theta} c_{2\downarrow} c_{2\uparrow} c_{1\downarrow} = n_{2\uparrow} c_{1\uparrow}^{\dagger} c_{2\downarrow} c_{1\downarrow}$$

$$\tilde{\phi}_{19} = c_{1\downarrow}^{\dagger} c_{2\uparrow}^{\dagger} I_{\theta} c_{2\downarrow} c_{1\downarrow} c_{1\uparrow} = n_{1\downarrow} c_{2\uparrow}^{\dagger} c_{2\downarrow} c_{1\uparrow}$$

$$\tilde{\phi}_{19_p} = -c_{1\uparrow}^{\dagger} c_{2\downarrow}^{\dagger} I_{\theta} c_{2\downarrow} c_{2\uparrow} c_{1\downarrow} = -n_{1\downarrow} c_{1\uparrow} c_{2\uparrow}^{\dagger} c_{1\downarrow}$$

$$\tilde{\phi}_{20} = c_{2\uparrow}^{\dagger} c_{2\downarrow}^{\dagger} I_{\theta} c_{2\downarrow} c_{1\downarrow} c_{1\uparrow} = n_{2\downarrow} c_{2\uparrow}^{\dagger} c_{1\downarrow} c_{1\uparrow}$$

$$\tilde{\phi}_{20_p} = c_{1\uparrow}^{\dagger} c_{1\downarrow}^{\dagger} I_{\theta} c_{2\downarrow} c_{2\uparrow} c_{1\downarrow} = n_{1\downarrow} c_{1\uparrow}^{\dagger} c_{2\downarrow} c_{2\uparrow}$$

$$\tilde{\phi}_{21} = c_{2\uparrow}^{\dagger} I_{\theta} c_{1\downarrow} c_{1\uparrow} = (1-n_{2\downarrow}) c_{2\uparrow}^{\dagger} c_{1\downarrow} c_{1\uparrow}$$

$$\tilde{\phi}_{21_p} = c_{1\uparrow}^{\dagger} I_{\theta} c_{2\downarrow} c_{2\uparrow} = (1-n_{1\downarrow}) c_{1\uparrow}^{\dagger} c_{2\downarrow} c_{2\uparrow}$$

$$\tilde{\phi}_{22} = c_{1\downarrow}^{\dagger} I_{\theta} c_{2\uparrow} c_{1\uparrow} = (1-n_{2\downarrow}) c_{1\downarrow}^{\dagger} c_{2\uparrow} c_{1\uparrow}$$

$$\tilde{\phi}_{22_p} = -c_{2\downarrow}^{\dagger} I_{\theta} c_{2\uparrow} c_{1\uparrow} = -(1-n_{1\downarrow}) c_{2\downarrow}^{\dagger} c_{2\uparrow} c_{1\uparrow}$$

$$\tilde{\phi}_{23} = c_{1\uparrow}^{\dagger} I_{\ominus} c_{2\uparrow} c_{1\downarrow} = \left(1 - n_{2\downarrow}\right) c_{1\uparrow}^{\dagger} c_{2\uparrow} c_{1\downarrow}$$

$$\tilde{\phi}_{23p} = -c_{2\uparrow}^{\dagger} I_{\ominus} c_{2\downarrow} c_{1\uparrow} = -\left(1 - n_{1\downarrow}\right) c_{2\uparrow}^{\dagger} c_{2\downarrow} c_{1\uparrow}$$

$$\tilde{\phi}_{24} = c_{1\uparrow}^{\dagger} I_{\ominus} c_{2\downarrow} c_{1\downarrow} = \left(1 - n_{2\uparrow}\right) c_{1\uparrow}^{\dagger} c_{2\downarrow} c_{1\downarrow}$$

$$\tilde{\phi}_{24p} = -c_{2\uparrow}^{\dagger} I_{\ominus} c_{2\downarrow} c_{1\downarrow} = -\left(1 - n_{1\uparrow}\right) c_{2\uparrow}^{\dagger} c_{2\downarrow} c_{1\downarrow}$$

Three-particle operators:

$$\phi_{1}^{(3)} = I_{\ominus} c_{2\uparrow} c_{1\downarrow} c_{1\uparrow} = \left(1 - n_{2\downarrow}\right) c_{2\uparrow} c_{1\downarrow} c_{1\uparrow}$$

$$\phi_{1p}^{(3)} = I_{\ominus} c_{2\downarrow} c_{2\uparrow} c_{1\uparrow} = \left(1 - n_{1\downarrow}\right) c_{2\downarrow} c_{2\uparrow} c_{1\uparrow}$$

$$\phi_{2}^{(3)} = I_{\ominus} c_{2\downarrow} c_{1\downarrow} c_{1\uparrow} = \left(1 - n_{2\uparrow}\right) c_{2\downarrow} c_{1\downarrow} c_{1\uparrow}$$

$$\phi_{2p}^{(3)} = I_{\ominus} c_{2\downarrow} c_{2\uparrow} c_{1\downarrow} = \left(1 - n_{1\uparrow}\right) c_{2\downarrow} c_{2\uparrow} c_{1\downarrow}$$

$$\phi_{1}^{(4)} = c_{1\uparrow}^{\dagger} I_{\ominus} c_{2\downarrow} c_{2\uparrow} c_{1\downarrow} c_{1\uparrow} = -n_{1\uparrow} c_{2\downarrow} c_{2\uparrow} c_{1\downarrow}$$

$$\phi_{1p}^{(4)} = c_{2\uparrow}^{\dagger} I_{\ominus} c_{2\downarrow} c_{2\uparrow} c_{1\downarrow} c_{1\uparrow} = -n_{2\uparrow} c_{2\downarrow} c_{1\downarrow} c_{1\uparrow}$$

$$\phi_{2}^{(4)} = c_{1\downarrow}^{\dagger} I_{\ominus} c_{2\downarrow} c_{2\uparrow} c_{1\downarrow} c_{1\uparrow} = n_{1\downarrow} c_{2\downarrow} c_{2\uparrow} c_{1\uparrow}$$

$$\phi_{2p}^{(4)} = c_{2\downarrow}^{\dagger} I_{\ominus} c_{2\downarrow} c_{2\uparrow} c_{1\downarrow} c_{1\uparrow} = n_{2\downarrow} c_{2\uparrow} c_{1\downarrow} c_{1\uparrow}$$

Orthogonal projection operators for the group U(16):

$$h_{0} = I_{\ominus}$$

$$h_{1} = c_{1\uparrow}^{\dagger} I_{\ominus} c_{1\uparrow}$$

$$h_2 = c_{1\downarrow}^\dagger I_\theta c_{1\downarrow}$$

$$h_3 = c_{2\uparrow}^\dagger I_\theta c_{2\uparrow}$$

$$h_4 = c_{2\downarrow}^\dagger I_\theta c_{2\downarrow}$$

$$h_5 = c_{1\uparrow}^\dagger c_{1\downarrow}^\dagger I_\theta c_{1\downarrow} c_{1\uparrow}$$

$$h_6 = c_{2\uparrow}^\dagger c_{2\downarrow}^\dagger I_\theta c_{2\downarrow} c_{2\uparrow}$$

$$h_7 = c_{1\uparrow}^\dagger c_{2\uparrow}^\dagger I_\theta c_{2\uparrow} c_{1\uparrow}$$

$$h_8 = c_{1\downarrow}^\dagger c_{2\uparrow}^\dagger I_\theta c_{2\uparrow} c_{1\downarrow}$$

$$h_9 = c_{1\uparrow}^\dagger c_{2\downarrow}^\dagger I_\theta c_{2\downarrow} c_{1\uparrow}$$

$$h_{10} = c_{1\downarrow}^\dagger c_{2\downarrow}^\dagger I_\theta c_{2\downarrow} c_{1\downarrow}$$

$$h_{11} = c_{1\uparrow}^\dagger c_{1\downarrow}^\dagger c_{2\uparrow}^\dagger I_\theta c_{2\uparrow} c_{1\downarrow} c_{1\uparrow}$$

$$h_{12} = c_{1\uparrow}^\dagger c_{2\uparrow}^\dagger c_{2\downarrow}^\dagger I_\theta c_{2\downarrow} c_{2\uparrow} c_{1\uparrow}$$

$$h_{13} = c_{1\uparrow}^\dagger c_{1\downarrow}^\dagger c_{2\downarrow}^\dagger I_\theta c_{2\downarrow} c_{1\downarrow} c_{1\uparrow}$$

$$h_{14} = c_{1\downarrow}^{\dagger} c_{2\uparrow}^{\dagger} c_{2\downarrow}^{\dagger} I_{\theta} c_{2\downarrow} c_{2\uparrow} c_{1\downarrow}$$

$$h_{15} = c_{1\uparrow}^{\dagger} c_{1\downarrow}^{\dagger} c_{2\uparrow}^{\dagger} c_{2\downarrow}^{\dagger} I_{\theta} c_{2\downarrow} c_{2\uparrow} c_{1\downarrow} c_{1\uparrow}$$

In order to operate with the Liouville operator on the Judd states we use the following relations:

$$H = H_0 + H_h$$

$$H_0 = \sum_{i,\sigma} \epsilon_{i,\sigma} n_{i,\sigma} + U \sum_i n_{i,\sigma} n_{i,-\sigma} \qquad \begin{array}{l} i = 1,2 \\ \sigma = \uparrow, \downarrow \end{array}$$

$$H_h = t \sum_{\sigma} \left(c_{1,\sigma}^{\dagger} c_{2,\sigma} + c_{2,\sigma}^{\dagger} c_{1,\sigma} \right)$$

$$L_0 \theta = [\theta, H_0] \;, \quad L_h \theta = [\theta, H_h] \;, \quad L = L_0 + L_h$$

$$L(ABC) = (LA)BC + A(LB)C + AB(LC)$$

$$L_0 c_{i,\sigma} = \epsilon_{i,\sigma} c_{i,\sigma} + U n_{i,-\sigma} c_{i,\sigma}$$

$$L_0 c_{i,\sigma}^{\dagger} = -\epsilon_{i,\sigma} c_{i,\sigma}^{\dagger} - U n_{i,-\sigma} c_{i,\sigma}^{\dagger}$$

$$L_0 n_{i,\sigma} = 0$$

$$L_h c_{i,\sigma} = t c_{i',\sigma} \;, \quad i' = i \pm 1$$

$$L_h c^{\dagger}_{i,\sigma} = -t c^{\dagger}_{i',\sigma} \quad , \quad i' = i \pm 1$$

$$L_h n_{i,\sigma} = t \left(c^{\dagger}_{i,\sigma} c_{i',\sigma} - c^{\dagger}_{i'\sigma} c_{i,\sigma} \right) \quad , \quad i' = i \pm 1$$

Notation: $\quad \phi_{i\pm} = \phi_i \pm \phi_{i\rho}$

$$L \phi_{9+} = \left(\epsilon + U + t \right) \phi_{9+}$$

$$L \phi_{9-} = \left(\epsilon + U - t \right) \phi_{9-}$$

$$L \phi_{10\pm} = \left(\epsilon \pm t \right) \phi_{10\pm}$$

$$L \left(\phi_{11\pm} - \tilde{\phi}_{20\pm} \right) = \left(\epsilon \pm t \right) \left(\phi_{11\pm} - \tilde{\phi}_{20\pm} \right)$$

$$L \left(\phi_{11\pm} + \tilde{\phi}_{20\pm} \right) = \left(\epsilon \mp t \right) \left(\phi_{11\pm} + \tilde{\phi}_{20\pm} \right) - 2t \left(\phi_{12\pm} - \tilde{\phi}_{19\pm} \right)$$

$$L \left(\phi_{12\pm} + \tilde{\phi}_{19\pm} \right) = \left(\epsilon + U \pm t \right) \left(\phi_{12\pm} + \tilde{\phi}_{19\pm} \right)$$

$$L \left(\phi_{12\pm} - \tilde{\phi}_{19\pm} \right) = \left(\epsilon + U \mp t \right) \left(\phi_{12\pm} - \tilde{\phi}_{19\pm} \right) - 2t \left(\phi_{11\pm} + \tilde{\phi}_{20\pm} \right)$$

$$L \left(\phi_{13\pm} \mp \tilde{\phi}_{21\pm} \right) = \left(\epsilon + U \pm t \right) \left(\phi_{13\pm} \mp \tilde{\phi}_{21\pm} \right)$$

$$L \left(\phi_{13\pm} \pm \tilde{\phi}_{21\pm} \right) = \left(\epsilon + U \mp t \right) \left(\phi_{13\pm} \pm \tilde{\phi}_{21\pm} \right) + 2t \left(\phi_{14\pm} - \tilde{\phi}_{23\pm} \right)$$

$$L\left(\phi_{14\pm} + \tilde{\phi}_{23\pm}\right) = \left(\epsilon \pm t\right)\left(\phi_{14\pm} + \tilde{\phi}_{23\pm}\right)$$

$$L\left(\phi_{14\pm} - \tilde{\phi}_{23\pm}\right) = \left(\epsilon \mp t\right)\left(\phi_{14\pm} - \tilde{\phi}_{23\pm}\right) + 2t\left(\phi_{13\pm} \pm \tilde{\phi}_{21\pm}\right)$$

$$L\phi_{15\pm} = \left(\epsilon \pm t\right)\phi_{15\pm}$$

$$L\phi_{16\pm} = \left(\epsilon \pm t\right)\phi_{16\pm}$$

$$L\tilde{\phi}_{17\pm} = \left(\epsilon + U \pm t\right)\tilde{\phi}_{17\pm}$$

$$L\tilde{\phi}_{18\pm} = \left(\epsilon + U \pm t\right)\tilde{\phi}_{18\pm}$$

$$L\tilde{\phi}_{22\pm} = \left(\epsilon \pm t\right)\tilde{\phi}_{22\pm}$$

$$L\tilde{\phi}_{24\pm} = \left(\epsilon \pm t\right)\tilde{\phi}_{24\pm}$$

$$L\phi_{1+}^{(3)} = \left(3\epsilon + U - t\right)\phi_{1+}^{(3)}$$

$$L\phi_{1-}^{(3)} = \left(3\epsilon + U - t\right)\phi_{1-}^{(3)}$$

$$L\phi_{2+}^{(3)} = \left(3\epsilon + U - t\right)\phi_{2+}^{(3)}$$

$$L\phi_{2-}^{(3)} = \left(3\epsilon + U - t\right)\phi_{2-}^{(3)}$$

$$L\phi_{1+}^{(4)} = \left(3\epsilon + 2U - t\right)\phi_{1+}^{(4)}$$

$$L\phi_{1-}^{(4)} = \left(3\epsilon + 2U - t\right)\phi_{1-}^{(4)}$$

$$L\phi_{2+}^{(4)} = \left(3\epsilon + 2U - t\right)\phi_{2+}^{(4)}$$

$$L\phi_{2-}^{(4)} = \left(3\epsilon + 2U - t\right)\phi_{2-}^{(4)}$$

Appendix B

We solve here for the inner products $\langle\!\langle \Psi_{i\pm}, \Psi_{i\pm} \rangle\!\rangle$. Since the eigen-functions Ψ_i are expressed in terms of the stepping operators ϕ, a preliminary step to the calculation of $\langle\!\langle \Psi_{i\pm}, \Psi_{i\pm} \rangle\!\rangle$ will be to calculate the non-vanishing $\langle\!\langle \phi_i, \phi_j \rangle\!\rangle$.

From the definition of the scalar product on the superspace and from the structure of the invariant I_θ we have:

$$\langle\!\langle \phi_i, \phi_j \rangle\!\rangle = \langle [\phi_j, \phi_i^\dagger]_+ \rangle$$
$$= \langle A_j^\dagger I_\theta A_j' A_i'^\dagger I_\theta A_i + A_i'^\dagger I_\theta A_i A_j^\dagger I_\theta A_j' \rangle = 0$$

$$\text{if} \quad i \neq j$$

Using site-exchange invariance i.e.

$$\langle n_{1\uparrow} c_{1\downarrow}^\dagger c_{2\downarrow} \rangle = \langle n_{2\uparrow} c_{2\downarrow}^\dagger c_{1\downarrow} \rangle$$

$$\langle n_{1\uparrow} n_{1\downarrow} n_{2\downarrow} \rangle = \langle n_{1\downarrow} n_{2\uparrow} n_{2\downarrow} \rangle$$

$$\text{etc.}$$

and spin-exchange invariance

$$\langle n_{1\uparrow} c_{1\downarrow}^\dagger c_{2\downarrow} \rangle = \langle n_{1\downarrow} c_{1\uparrow}^\dagger c_{2\uparrow} \rangle$$

$$\langle c_{1\uparrow}^\dagger c_{2\uparrow} \rangle = \langle c_{1\downarrow}^\dagger c_{2\downarrow} \rangle$$

$$\text{etc.}$$

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and the definition

$$\left(\!\!\left(\phi_{ip}, \phi_{jp}\right)\!\!\right) = \left\langle P\left[\phi_{jp}, \phi_{ip}\right]P^{-1}\right\rangle = \left(\!\!\left(\phi_i, \phi_j\right)\!\!\right)$$

the following relations are true:

$$\left(\!\!\left(\phi_i, \phi_i\right)\!\!\right) = \left(\!\!\left(\phi_{ip}, \phi_{ip}\right)\!\!\right)$$

$$\left(\!\!\left(\phi_i, \phi_{jp}\right)\!\!\right) = \left(\!\!\left(\phi_{ip}, \tilde{\phi}_j\right)\!\!\right)$$

$$\left(\!\!\left(\tilde{\phi}_i, \phi_i\right)\!\!\right) = \left(\!\!\left(\phi_i, \tilde{\phi}_i\right)\!\!\right)$$

$$\left(\!\!\left(\phi_i, \phi_i\right)\!\!\right) = \left(\!\!\left(\tilde{\phi}_i, \tilde{\phi}_i\right)\!\!\right)$$

We then have the non-vanishing expressions:

$$\left(\!\!\left(\phi_1, \phi_1\right)\!\!\right) = \left(\!\!\left(\phi_{1p}, \phi_{1p}\right)\!\!\right) = \left\langle \left(1 - n_{1\downarrow}\right)\left(1 - n_{2\downarrow}\right)\left(1 - n_{2\uparrow}\right)\right\rangle$$

$$\left(\!\!\left(\phi_2, \phi_2\right)\!\!\right) = \left(\!\!\left(\phi_{2p}, \phi_{2p}\right)\!\!\right) = \left\langle \left(1 - n_{2\uparrow}\right)\left(1 - n_{2\downarrow}\right)n_{1\downarrow}\right\rangle$$

$$\left(\!\!\left(\phi_3, \phi_3\right)\!\!\right) = \left(\!\!\left(\phi_{3p}, \phi_{3p}\right)\!\!\right) = \left\langle \left(1 - n_{1\downarrow}\right)\left(1 - n_{2\downarrow}\right)n_{2\uparrow}\right\rangle$$

$$\left(\!\!\left(\phi_4, \phi_4\right)\!\!\right) = \left(\!\!\left(\phi_{4p}, \phi_{4p}\right)\!\!\right) = \left\langle \left(1 - n_{1\downarrow}\right)\left(1 - n_{2\uparrow}\right)n_{2\downarrow}\right\rangle$$

$$\left(\!\left(\phi_5, \phi_5\right)\!\right) = \left(\!\left(\phi_{5P}, \phi_{5P}\right)\!\right) = \left\langle \left(1-n_{2\downarrow}\right) n_{2\uparrow} n_{1\downarrow} \right\rangle$$

$$\left(\!\left(\phi_6, \phi_6\right)\!\right) = \left(\!\left(\phi_{6P}, \phi_{6P}\right)\!\right) = \left\langle \left(1-n_{2\uparrow}\right) n_{2\downarrow} n_{1\downarrow} \right\rangle$$

$$\left(\!\left(\phi_7, \phi_7\right)\!\right) = \left(\!\left(\phi_{7P}, \phi_{7P}\right)\!\right) = \left\langle \left(1-n_{1\downarrow}\right) n_{2\downarrow} n_{2\uparrow} \right\rangle$$

$$\left(\!\left(\phi_8, \phi_8\right)\!\right) = \left(\!\left(\phi_{8P}, \phi_{8P}\right)\!\right) = \left\langle n_{2\downarrow} n_{2\uparrow} n_{1\downarrow} \right\rangle$$

$$\left(\!\left(\phi_1, \phi_{1P}\right)\!\right) = \left\langle \left(1-n_{1\downarrow}\right)\left(1-n_{2\downarrow}\right) c_{1\uparrow}^{\dagger} c_{2\uparrow} \right\rangle = \left(\!\left(\phi_{1P}, \phi_1\right)\!\right)$$

$$\left(\!\left(\phi_3, \phi_{3P}\right)\!\right) = \left\langle \left(1-n_{1\downarrow}\right)\left(1-n_{2\downarrow}\right) c_{1\uparrow}^{\dagger} c_{2\uparrow} \right\rangle = \left(\!\left(\phi_{3P}, \phi_3\right)\!\right)$$

$$\left(\!\left(\phi_6, \phi_{6P}\right)\!\right) = \left\langle n_{2\downarrow} n_{1\downarrow} c_{1\uparrow}^{\dagger} c_{2\uparrow} \right\rangle = \left(\!\left(\phi_{6P}, \phi_6\right)\!\right)$$

$$\left(\!\left(\phi_8, \phi_{8P}\right)\!\right) = -\left\langle n_{2\downarrow} n_{1\downarrow} c_{1\uparrow}^{\dagger} c_{2\uparrow} \right\rangle = \left(\!\left(\phi_{8P}, \phi_8\right)\!\right)$$

$$\left(\!\left(\phi_2, \tilde{\phi}_2\right)\!\right) = \left(\!\left(\tilde{\phi}_2, \phi_2\right)\!\right) = \left\langle \left(1-n_{1\uparrow}\right)\left(1-n_{2\uparrow}\right) c_{1\downarrow}^{\dagger} c_{2\downarrow} \right\rangle$$

$$\left(\!\left(\phi_2, \tilde{\phi}_{2P}\right)\!\right) = \left(\!\left(\tilde{\phi}_2, \phi_{2P}\right)\!\right) = \left\langle c_{2\uparrow}^{\dagger} c_{2\downarrow}^{\dagger} c_{1\downarrow} c_{1\uparrow} \right\rangle$$

$$\left(\!\left(\phi_4, \tilde{\phi}_4\right)\!\right) = \left(\!\left(\tilde{\phi}_4, \phi_4\right)\!\right) = \left(\!\left(\phi_2, \tilde{\phi}_2\right)\!\right) = \left(\!\left(\tilde{\phi}_2, \phi_2\right)\!\right) = \left\langle \left(1-n_{1\uparrow}\right)\left(1-n_{2\uparrow}\right) c_{1\downarrow}^{\dagger} c_{2\downarrow} \right\rangle$$

$$\left(\!\left(\phi_4, \tilde{\phi}_{4P}\right)\!\right) = \left(\!\left(\tilde{\phi}_4, \phi_{4P}\right)\!\right) = \left\langle c_{1\uparrow}^{\dagger} c_{2\downarrow}^{\dagger} c_{1\downarrow} c_{2\uparrow} \right\rangle$$

$$\left(\!\left(\phi_2, \tilde{\phi}_4\right)\!\right) = \left(\!\left(\phi_4, \tilde{\phi}_2\right)\!\right) = \left\langle \left(1-n_{2\uparrow}\right) n_{1\uparrow} c_{1\downarrow}^{\dagger} c_{2\downarrow} \right\rangle$$

$$\langle\!\langle \phi_2 , \phi_{4P} \rangle\!\rangle = \langle (1-n_{2\downarrow}) n_{1\downarrow} c_{1\uparrow}^\dagger c_{2\uparrow} \rangle$$

$$\langle\!\langle \phi_4 , \phi_{2P} \rangle\!\rangle = \langle\!\langle \phi_2 , \phi_{4P} \rangle\!\rangle = \langle (1-n_{1\downarrow}) n_{2\downarrow} c_{1\uparrow}^\dagger c_{2\uparrow} \rangle$$

$$\langle\!\langle \phi_7 , \tilde{\phi}_7 \rangle\!\rangle = -\langle n_{1\uparrow} n_{2\uparrow} c_{1\downarrow}^\dagger c_{2\downarrow} \rangle$$

$$\langle\!\langle \phi_7 , \tilde{\phi}_{7P} \rangle\!\rangle = \langle c_{1\uparrow}^\dagger c_{1\downarrow}^\dagger c_{2\downarrow} c_{2\uparrow} \rangle$$

$$\langle\!\langle \phi_5 , \phi_5 \rangle\!\rangle = -\langle n_{1\uparrow} n_{2\uparrow} c_{1\downarrow}^\dagger c_{2\downarrow} \rangle$$

$$\langle\!\langle \phi_5 , \phi_{5P} \rangle\!\rangle = \langle c_{2\downarrow}^\dagger c_{1\uparrow}^\dagger c_{2\uparrow} c_{1\downarrow} \rangle$$

$$\langle\!\langle \phi_5 , \phi_{7P} \rangle\!\rangle = \langle\!\langle \tilde{\phi}_5 , \tilde{\phi}_{7P} \rangle\!\rangle = -\langle\!\langle \phi_2 , \phi_{4P} \rangle\!\rangle$$

$$= \langle\!\langle \phi_5 , \tilde{\phi}_7 \rangle\!\rangle = \langle\!\langle \phi_{2P} , \tilde{\phi}_{4P} \rangle\!\rangle$$

$$= -\langle (1-n_{1\downarrow}) n_{2\downarrow} c_{1\uparrow}^\dagger c_{2\uparrow} \rangle$$

We may now calculate the $\langle\!\langle \psi_i , \psi_i \rangle\!\rangle$.

$$\langle\!\langle \psi_{1\uparrow} , \psi_{1\uparrow} \rangle\!\rangle = 2\langle (1-n_{1\downarrow})(1-n_{2\uparrow})(1-n_{2\downarrow}) + (1-n_{1\downarrow})(1-n_{2\downarrow}) c_{1\uparrow}^\dagger c_{2\uparrow} \rangle$$

$$\langle\!\langle \psi_{1\downarrow} , \psi_{1\downarrow} \rangle\!\rangle = 2\langle (1-n_{1\downarrow})(1-n_{2\uparrow})(1-n_{2\downarrow}) - (1-n_{1\downarrow})(1-n_{2\downarrow}) c_{1\uparrow}^\dagger c_{2\uparrow} \rangle$$

$$\langle\!\langle \Psi_{2\pm}, \Psi_{2\pm}\rangle\!\rangle = 4\Big\langle (1-n_{2\uparrow})(1-n_{2\downarrow})n_{1\downarrow} \mp (1-n_{1\uparrow})(1-n_{2\uparrow})c_{2\downarrow}^{\dagger}c_{1\downarrow} - c_{1\uparrow}^{\dagger}c_{1\downarrow}^{\dagger}c_{2\downarrow}c_{2\uparrow}\Big\rangle$$

$$\langle\!\langle \Psi_{3\pm}, \Psi_{3\pm}\rangle\!\rangle = 2\Big\langle (1-n_{1\downarrow})(1-n_{2\downarrow})n_{2\uparrow} \mp (1-n_{1\downarrow})(1-n_{2\downarrow})c_{1\uparrow}^{\dagger}c_{2\uparrow}\Big\rangle$$

$$\langle\!\langle \Psi_{4\pm}, \Psi_{4\pm}\rangle\!\rangle = 4\Big\langle (1-n_{1\downarrow})(1-n_{2\uparrow})n_{2\downarrow} \mp (1-n_{1\uparrow})(1-n_{2\uparrow})c_{1\downarrow}^{\dagger}c_{2\downarrow} - c_{1\uparrow}^{\dagger}c_{2\downarrow}^{\dagger}c_{1\downarrow}c_{2\uparrow}\Big\rangle$$

$$\langle\!\langle \Psi_{5\pm}, \Psi_{5\pm}\rangle\!\rangle = 4\Big\langle (1-n_{2\downarrow})n_{2\uparrow}n_{1\downarrow} \pm n_{1\uparrow}n_{2\uparrow}c_{1\downarrow}^{\dagger}c_{2\downarrow} - c_{2\downarrow}^{\dagger}c_{1\uparrow}^{\dagger}c_{2\uparrow}c_{1\downarrow}\Big\rangle$$

$$\langle\!\langle \Psi_{6\pm}, \Psi_{6\pm}\rangle\!\rangle = 2\Big\langle (1-n_{2\uparrow})n_{2\downarrow}n_{1\downarrow} \pm n_{2\downarrow}n_{1\downarrow}c_{1\uparrow}^{\dagger}c_{2\uparrow}\Big\rangle$$

$$\langle\!\langle \Psi_{7\pm}, \Psi_{7\pm}\rangle\!\rangle = 4\Big\langle (1-n_{1\downarrow})n_{2\downarrow}n_{2\uparrow} \pm n_{1\uparrow}n_{2\uparrow}c_{1\downarrow}^{\dagger}c_{2\downarrow} - c_{1\uparrow}^{\dagger}c_{1\downarrow}^{\dagger}c_{2\downarrow}c_{2\uparrow}\Big\rangle$$

$$\langle\!\langle \Psi_{8\pm}, \Psi_{8\pm}\rangle\!\rangle = 2\Big\langle n_{2\downarrow}n_{2\uparrow}n_{1\downarrow} \mp n_{2\downarrow}n_{1\downarrow}c_{1\uparrow}^{\dagger}c_{2\uparrow}\Big\rangle$$

$$\langle\!\langle \Psi_{2\pm}^{(1)}, \Psi_{2\pm}^{(1)}\rangle\!\rangle = 4\alpha_1^2\Big\langle (1-n_{2\uparrow})(1-n_{2\downarrow})n_{1\downarrow} \pm (1-n_{1\uparrow})(1-n_{2\uparrow})c_{1\downarrow}^{\dagger}c_{2\downarrow} + c_{2\uparrow}^{\dagger}c_{2\downarrow}^{\dagger}c_{1\downarrow}c_{1\uparrow}\Big\rangle$$

$$+\, 4\beta_1^2\Big\langle (1-n_{1\downarrow})(1-n_{2\uparrow})n_{2\downarrow} \pm (1-n_{1\uparrow})(1-n_{2\uparrow})c_{1\downarrow}^{\dagger}c_{2\downarrow} + c_{1\uparrow}^{\dagger}c_{2\downarrow}^{\dagger}c_{1\downarrow}c_{2\uparrow}\Big\rangle$$

$$+\, 8\alpha_1\beta_1\Big\langle (1-n_{1\downarrow})n_{2\downarrow}c_{1\uparrow}^{\dagger}c_{2\uparrow} + (1-n_{2\downarrow})n_{1\downarrow}c_{1\uparrow}^{\dagger}c_{2\uparrow}\Big\rangle$$

$$\left(\!\!\left(\psi_{2\pm}^{(2)},\psi_{2\pm}^{(2)}\right)\!\!\right)=4\alpha_2^2\left\langle\!\!\left\langle\left(1-n_{2\uparrow}\right)\left(1-n_{2\downarrow}\right)n_{1\downarrow}\pm\left(1-n_{1\uparrow}\right)\left(1-n_{2\uparrow}\right)c_{1\downarrow}^{\dagger}c_{2\downarrow}+c_{2\uparrow}^{\dagger}c_{2\downarrow}^{\dagger}c_{1\downarrow}c_{1\uparrow}\right\rangle\!\!\right\rangle$$

$$+4\beta_2^2\left\langle\!\!\left\langle\left(1-n_{1\downarrow}\right)\left(1-n_{2\uparrow}\right)n_{2\downarrow}\pm\left(1-n_{1\uparrow}\right)\left(1-n_{2\uparrow}\right)c_{1\downarrow}^{\dagger}c_{2\downarrow}+c_{1\uparrow}^{\dagger}c_{2\downarrow}^{\dagger}c_{1\downarrow}c_{2\uparrow}\right\rangle\!\!\right\rangle$$

$$+8\alpha_2\beta_2\left\langle\!\!\left\langle\left(1-n_{1\downarrow}\right)n_{2\downarrow}c_{1\uparrow}^{\dagger}c_{2\uparrow}+\left(1-n_{2\downarrow}\right)n_{1\downarrow}c_{1\uparrow}^{\dagger}c_{2\uparrow}\right\rangle\!\!\right\rangle$$

$$\left(\!\!\left(\psi_{5\pm}^{(1)},\psi_{5\pm}^{(1)}\right)\!\!\right)=4\alpha_1^2\left\langle\!\!\left\langle\left(1-n_{1\downarrow}\right)n_{2\downarrow}n_{1\uparrow}\mp n_{1\downarrow}n_{2\downarrow}c_{1\uparrow}^{\dagger}c_{2\uparrow}+c_{1\downarrow}^{\dagger}c_{2\downarrow}c_{2\uparrow}^{\dagger}c_{1\uparrow}\right\rangle\!\!\right\rangle$$

$$+4\beta_1^2\left\langle\!\!\left\langle\left(1-n_{1\downarrow}\right)n_{2\downarrow}n_{2\uparrow}\mp n_{1\downarrow}n_{2\downarrow}c_{1\uparrow}^{\dagger}c_{2\uparrow}+c_{1\downarrow}^{\dagger}c_{2\downarrow}c_{1\uparrow}^{\dagger}c_{2\uparrow}\right\rangle\!\!\right\rangle$$

$$-8\alpha_1\beta_1\left\langle\!\!\left\langle\left(n_{1\downarrow}+n_{2\downarrow}-2n_{1\downarrow}n_{2\downarrow}\right)c_{1\uparrow}^{\dagger}c_{2\uparrow}\right\rangle\!\!\right\rangle$$

$$\left(\!\!\left(\psi_{5\pm}^{(2)},\psi_{5\pm}^{(2)}\right)\!\!\right)=4\alpha_2^2\left\langle\!\!\left\langle\left(1-n_{1\downarrow}\right)n_{2\downarrow}n_{1\uparrow}\mp n_{1\downarrow}n_{2\downarrow}c_{1\uparrow}^{\dagger}c_{2\uparrow}+c_{1\downarrow}^{\dagger}c_{2\downarrow}c_{2\uparrow}^{\dagger}c_{1\uparrow}\right\rangle\!\!\right\rangle$$

$$+4\beta_2^2\left\langle\!\!\left\langle\left(1-n_{1\downarrow}\right)n_{2\downarrow}n_{2\uparrow}\mp n_{1\downarrow}n_{2\downarrow}c_{1\uparrow}^{\dagger}c_{2\uparrow}+c_{1\downarrow}^{\dagger}c_{2\downarrow}c_{1\uparrow}^{\dagger}c_{2\uparrow}\right\rangle\!\!\right\rangle$$

$$-8\alpha_2\beta_2\left\langle\!\!\left\langle\left(n_{1\downarrow}+n_{2\downarrow}-2n_{1\downarrow}n_{2\downarrow}\right)c_{1\uparrow}^{\dagger}c_{2\uparrow}\right\rangle\!\!\right\rangle$$

Appendix C

Using the dispersion relation

$$\left\langle \psi_i^\dagger \, \psi_i \right\rangle = \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \, f_0(\omega) \, \mathcal{I}m \, \left(\!\!\left(\psi_i \, , \, (\omega - i\delta - L)^{-1} \, \psi_i \right)\!\!\right)$$

which for $L\psi_i = \lambda_i \psi_i$ simplifies to

$$\left\langle \psi_i^\dagger \, \psi_i \right\rangle = \left(\!\!\left(\psi_i \, , \, \psi_i \right)\!\!\right) f_0(\lambda_i)$$

with $\quad f_0(\lambda_i) = \left(\epsilon^{\beta(\lambda_i - \mu)} + 1 \right)^{-1}$

we have the following relations:

$$\left\langle \psi_{1\pm}^\dagger \, \psi_{1\pm} \right\rangle = \left\langle (1 - n_{1\downarrow})(1 - n_{2\downarrow}) \left\{ 2 - n_{1\uparrow} - n_{2\uparrow} \pm \left(c_{1\uparrow}^\dagger c_{2\uparrow} + c_{2\uparrow}^\dagger c_{1\uparrow} \right) \right\} \right\rangle f_0(\epsilon \pm t)$$

$$= \left\langle (1 - n_{1\downarrow})(1 - n_{2\downarrow}) \left\{ n_{1\uparrow} + n_{2\uparrow} - 2 n_{1\uparrow} n_{2\uparrow} \pm \left(c_{1\uparrow}^\dagger c_{2\uparrow} + c_{2\uparrow}^\dagger c_{1\uparrow} \right) \right\} \right\rangle$$

$$\left\langle \psi_{2\pm}^\dagger \, \psi_{2\pm} \right\rangle = 4 \left\langle (1 - n_{1\downarrow}) n_{2\downarrow} (1 - n_{1\uparrow}) \mp (1 - n_{1\downarrow})(1 - n_{2\downarrow}) c_{1\uparrow}^\dagger c_{2\uparrow} - c_{1\downarrow}^\dagger c_{2\downarrow} c_{1\uparrow}^\dagger c_{2\uparrow} \right\rangle f_0(\epsilon + U \pm t)$$

$$= 4 \left\langle (1 - n_{1\downarrow}) n_{2\downarrow} (1 - n_{1\uparrow}) n_{2\uparrow} - c_{1\downarrow}^\dagger c_{2\downarrow} - c_{1\uparrow}^\dagger c_{2\uparrow} \right.$$

$$\left\langle \psi_{3\pm}^\dagger \, \psi_{3\pm} \right\rangle = \left\langle (1 - n_{1\downarrow})(1 - n_{2\downarrow}) \left\{ n_{1\uparrow} + n_{2\uparrow} \mp \left(c_{1\uparrow}^\dagger c_{2\uparrow} + c_{2\uparrow}^\dagger c_{1\uparrow} \right) \right\} \right\rangle f_0(\epsilon \pm t)$$

$$= 2 \left\langle (1 - n_{1\downarrow})(1 - n_{2\downarrow}) n_{1\uparrow} n_{2\uparrow} \right\rangle$$

$$\langle \psi^\dagger_{4\pm} \psi_{4\pm} \rangle = 4 \left\langle (1-n_{1\downarrow}) n_{2\downarrow} (1-n_{2\uparrow}) \mp (1-n_{1\downarrow})(1-n_{2\downarrow}) c^\dagger_{1\uparrow} c_{2\uparrow} - c^\dagger_{1\downarrow} c_{2\downarrow} c^\dagger_{2\uparrow} c_{1\uparrow} \right\rangle f_0(\epsilon \pm t)$$

$$= 4 \left\langle (1-n_{1\downarrow}) n_{2\downarrow} (1-n_{2\uparrow}) n_{1\uparrow} - c^\dagger_{1\downarrow} c_{2\downarrow} c^\dagger_{2\uparrow} c_{1\uparrow} \right\rangle$$

$$\langle \psi^\dagger_{5\pm} \psi_{5\pm} \rangle = 4 \left\langle (1-n_{1\downarrow}) n_{2\downarrow} n_{1\uparrow} \pm n_{1\downarrow} n_{2\downarrow} c^\dagger_{1\uparrow} c_{2\uparrow} - c^\dagger_{1\downarrow} c_{2\downarrow} c^\dagger_{2\uparrow} c_{1\uparrow} \right\rangle f_0(\epsilon + U \pm t)$$

$$= 4 \left\langle (1-n_{1\downarrow}) n_{2\downarrow} n_{2\uparrow} n_{1\uparrow} \pm n_{1\downarrow} n_{2\downarrow} c^\dagger_{1\uparrow} c_{2\uparrow} \right\rangle$$

$$\langle \psi^\dagger_{6\pm} \psi_{6\pm} \rangle = \left\langle n_{1\downarrow} n_{2\downarrow} \left\{ 2 - n_{1\uparrow} - n_{2\uparrow} \pm (c^\dagger_{1\uparrow} c_{2\uparrow} + c^\dagger_{2\uparrow} c_{1\uparrow}) \right\} \right\rangle f_0(\epsilon + U \pm t)$$

$$= \left\langle n_{1\downarrow} n_{2\downarrow} \left\{ n_{1\uparrow} + n_{2\uparrow} - 2 n_{1\uparrow} n_{2\uparrow} \pm (c^\dagger_{1\uparrow} c_{2\uparrow} + c^\dagger_{2\uparrow} c_{1\uparrow}) \right\} \right\rangle$$

$$\langle \psi^\dagger_{7\pm} \psi_{7\pm} \rangle = 4 \left\langle (1-n_{1\downarrow}) n_{2\downarrow} n_{2\uparrow} \pm n_{1\downarrow} n_{2\downarrow} c^\dagger_{1\uparrow} c_{2\uparrow} - c^\dagger_{1\downarrow} c_{2\downarrow} c^\dagger_{1\uparrow} c_{2\uparrow} \right\rangle f_0(\epsilon \pm t)$$

$$= 4 \left\langle (1-n_{1\downarrow}) n_{2\downarrow} n_{2\uparrow} n_{1\uparrow} \pm n_{1\downarrow} n_{2\downarrow} c^\dagger_{1\uparrow} c_{2\uparrow} \right\rangle$$

$$\langle \psi^\dagger_{8\pm} \psi_{8\pm} \rangle = \left\langle n_{1\downarrow} n_{2\downarrow} \left\{ n_{1\uparrow} + n_{2\uparrow} \mp (c^\dagger_{1\uparrow} c_{2\uparrow} + c^\dagger_{2\uparrow} c_{1\uparrow}) \right\} \right\rangle f_0(\epsilon + U \pm t)$$

$$= 2 \left\langle n_{1\downarrow} n_{2\downarrow} n_{1\uparrow} n_{2\uparrow} \right\rangle$$

$$\langle \psi_{2\pm}^{1\dagger} \psi_{2\pm}^{1} \rangle = \Big\{ 4\alpha_1^2 \langle (1-n_{1\downarrow})n_{2\downarrow}(1-n_{1\uparrow}) \pm (1-n_{1\downarrow})(1-n_{2\downarrow})c_{1\uparrow}^{\dagger}c_{2\uparrow} + c_{1\downarrow}^{\dagger}c_{2\downarrow}c_{1\uparrow}^{\dagger}c_{2\uparrow} \rangle$$

$$+ 4\beta_1^2 \langle (1-n_{1\downarrow})n_{2\downarrow}(1-n_{2\uparrow}) \pm (1-n_{1\downarrow})(1-n_{2\downarrow})c_{1\uparrow}^{\dagger}c_{2\uparrow} + c_{1\downarrow}^{\dagger}c_{2\downarrow}c_{2\uparrow}^{\dagger}c_{1\uparrow} \rangle$$

$$+ 8\alpha_1\beta_1 \langle (n_{1\downarrow}+n_{2\downarrow}-2n_{1\downarrow}n_{2\downarrow})c_{1\uparrow}^{\dagger}c_{2\uparrow} \rangle \Big\} \, f_0(\lambda_{1\pm})$$

$$= 4\alpha_1^2 \langle (1-n_{1\downarrow})n_{2\downarrow}(1-n_{1\uparrow})n_{2\uparrow} + c_{1\downarrow}^{\dagger}c_{2\downarrow}c_{1\uparrow}^{\dagger}c_{2\uparrow} \rangle$$

$$+ 4\beta_1^2 \langle (1-n_{1\downarrow})n_{2\downarrow}(1-n_{2\uparrow})n_{1\uparrow}c_{1\downarrow}^{\dagger}c_{2\downarrow}c_{2\uparrow}^{\dagger}c_{1\uparrow} \rangle$$

$$+ 8\alpha_1\beta_1 \langle (n_{1\downarrow}+n_{2\downarrow}-2n_{1\downarrow}n_{2\downarrow})c_{1\uparrow}^{\dagger}c_{2\uparrow} \rangle$$

$$\langle \psi_{2\pm}^{2\dagger} \psi_{2\pm}^{2} \rangle = \Big\{ 4\alpha_2^2 \langle (1-n_{1\downarrow})n_{2\downarrow}(1-n_{1\uparrow}) \pm (1-n_{1\downarrow})(1-n_{2\downarrow})c_{1\uparrow}^{\dagger}c_{2\uparrow} + c_{1\downarrow}^{\dagger}c_{2\downarrow}c_{1\uparrow}^{\dagger}c_{2\uparrow} \rangle$$

$$+ 4\beta_2^2 \langle (1-n_{1\downarrow})n_{2\downarrow}(1-n_{2\uparrow}) \pm (1-n_{1\downarrow})(1-n_{2\downarrow})c_{1\uparrow}^{\dagger}c_{2\uparrow} + c_{1\downarrow}^{\dagger}c_{2\downarrow}c_{2\uparrow}^{\dagger}c_{1\uparrow} \rangle$$

$$+ 8\alpha_2\beta_2 \langle (n_{1\downarrow}+n_{2\downarrow}-2n_{1\downarrow}n_{2\downarrow})c_{1\uparrow}^{\dagger}c_{2\uparrow} \rangle \Big\} \, f_0(\lambda_{2\pm})$$

$$= 4\alpha_2^2 \langle (1-n_{1\downarrow})n_{2\downarrow}(1-n_{1\uparrow})n_{2\uparrow} + c_{1\downarrow}^{\dagger}c_{2\downarrow}c_{1\uparrow}^{\dagger}c_{2\uparrow} \rangle$$

$$+ 4\beta_2^2 \langle (1-n_{1\downarrow})n_{2\downarrow}(1-n_{2\uparrow})n_{1\uparrow}c_{1\downarrow}^{\dagger}c_{2\downarrow}c_{2\uparrow}^{\dagger}c_{1\uparrow} \rangle$$

$$+ 8\alpha_2\beta_2 \langle (n_{1\downarrow}+n_{2\downarrow}-2n_{1\downarrow}n_{2\downarrow})c_{1\uparrow}^{\dagger}c_{2\uparrow} \rangle$$

$$\langle \psi^{1\dagger}_{s\pm} \psi^{1}_{s\pm} \rangle = \Big\{ 4\alpha_1^2 \langle (1-n_{1\downarrow})n_{2\downarrow}n_{1\uparrow} \mp n_{1\downarrow}n_{2\downarrow} c^{\dagger}_{1\uparrow}c_{2\uparrow} + c^{\dagger}_{1\downarrow}c_{2\downarrow}c^{\dagger}_{2\uparrow}c_{1\uparrow} \rangle$$

$$+ 4\beta_1^2 \langle (1-n_{1\downarrow})n_{2\downarrow}n_{2\uparrow} \mp n_{1\downarrow}n_{2\downarrow} c^{\dagger}_{1\uparrow}c_{2\uparrow} + c^{\dagger}_{1\downarrow}c_{2\downarrow}c^{\dagger}_{1\uparrow}c_{2\uparrow} \rangle$$

$$- 8\alpha_1\beta_1 \langle (n_{1\downarrow}+n_{2\downarrow}-2n_{1\downarrow}n_{2\downarrow}) c^{\dagger}_{1\uparrow}c_{2\uparrow} \rangle \Big\} f_0(\lambda_{1\pm})$$

$$= 4\alpha_1^2 \langle (1-n_{1\downarrow})n_{2\downarrow}n_{2\uparrow}n_{1\uparrow} \mp n_{1\downarrow}n_{2\downarrow} c^{\dagger}_{1\uparrow}c_{2\uparrow} \rangle$$

$$+ 4\beta_1^2 \langle (1-n_{1\downarrow})n_{2\downarrow}n_{2\uparrow}n_{1\uparrow} \mp n_{1\downarrow}n_{2\downarrow} c^{\dagger}_{1\uparrow}c_{2\uparrow} \rangle$$

$$\langle \psi^{2\dagger}_{s\pm} \psi^{2}_{s\pm} \rangle = \Big\{ 4\alpha_2^2 \langle (1-n_{1\downarrow})n_{2\downarrow}n_{1\uparrow} \mp n_{1\downarrow}n_{2\downarrow} c^{\dagger}_{1\uparrow}c_{2\uparrow} + c^{\dagger}_{1\downarrow}c_{2\downarrow}c^{\dagger}_{2\uparrow}c_{1\uparrow} \rangle$$

$$+ 4\beta_2^2 \langle (1-n_{1\downarrow})n_{2\downarrow}n_{2\uparrow} \mp n_{1\downarrow}n_{2\downarrow} c^{\dagger}_{1\uparrow}c_{2\uparrow} + c^{\dagger}_{1\downarrow}c_{2\downarrow}c^{\dagger}_{1\uparrow}c_{2\uparrow} \rangle$$

$$- 8\alpha_2\beta_2 \langle (n_{1\downarrow}+n_{2\downarrow}-2n_{1\downarrow}n_{2\downarrow}) c^{\dagger}_{1\uparrow}c_{2\uparrow} \rangle \Big\} f_0(\lambda_{2\pm})$$

$$= 4\alpha_2^2 \langle (1-n_{1\downarrow})n_{2\downarrow}n_{2\uparrow}n_{1\uparrow} \mp n_{1\downarrow}n_{2\downarrow} c^{\dagger}_{1\uparrow}c_{2\uparrow} \rangle$$

$$+ 4\beta_2^2 \langle (1-n_{1\downarrow})n_{2\downarrow}n_{2\uparrow}n_{1\uparrow} \mp n_{1\downarrow}n_{2\downarrow} c^{\dagger}_{1\uparrow}c_{2\uparrow} \rangle$$

The dispersion relation arising from the off-diagonal Green

-function is given by:

$$4\langle c_{1\uparrow}^{\dagger} c_{2\uparrow}\rangle = (2 - 3\langle n_{1\uparrow}\rangle + \langle n_{1\uparrow} n_{2\uparrow}\rangle - \langle c_{1\downarrow}^{\dagger} c_{2\downarrow} c_{1\uparrow}^{\dagger} c_{2\uparrow}\rangle - \langle c_{1\downarrow}^{\dagger} c_{2\downarrow} c_{2\uparrow}^{\dagger} c_{1\uparrow}\rangle$$
$$- \langle c_{1\uparrow}^{\dagger} c_{2\uparrow}\rangle + \langle n_{1\downarrow} c_{1\uparrow}^{\dagger} c_{2\uparrow}\rangle + \langle n_{2\downarrow} c_{1\uparrow}^{\dagger} c_{2\uparrow}\rangle) f_{+}$$

$$- (2 - 3\langle n_{1\uparrow}\rangle + \langle n_{1\uparrow} n_{2\uparrow}\rangle - \langle c_{1\downarrow}^{\dagger} c_{2\downarrow} c_{1\uparrow}^{\dagger} c_{2\uparrow}\rangle - \langle c_{1\downarrow}^{\dagger} c_{2\downarrow} c_{2\uparrow}^{\dagger} c_{1\uparrow}\rangle$$
$$- \langle c_{1\uparrow}^{\dagger} c_{2\uparrow}\rangle + \langle n_{1\downarrow} c_{1\uparrow}^{\dagger} c_{2\uparrow}\rangle + \langle n_{2\downarrow} c_{1\uparrow}^{\dagger} c_{2\uparrow}\rangle) f_{-}$$

$$+ (\langle n_{1\uparrow}\rangle + \langle n_{1\uparrow} n_{2\uparrow}\rangle - \langle c_{1\downarrow}^{\dagger} c_{2\downarrow} c_{1\uparrow}^{\dagger} c_{2\uparrow}\rangle - \langle c_{1\downarrow}^{\dagger} c_{2\downarrow} c_{2\uparrow}^{\dagger} c_{1\uparrow}\rangle$$
$$- \langle c_{1\uparrow}^{\dagger} c_{2\uparrow}\rangle + \langle n_{1\downarrow} c_{1\uparrow}^{\dagger} c_{2\uparrow}\rangle + \langle n_{2\downarrow} c_{1\uparrow}^{\dagger} c_{2\uparrow}\rangle) \bar{f}_{+}$$

$$- (\langle n_{1\uparrow}\rangle + \langle n_{1\uparrow} n_{2\uparrow}\rangle - \langle c_{1\downarrow}^{\dagger} c_{2\downarrow} c_{1\uparrow}^{\dagger} c_{2\uparrow}\rangle - \langle c_{1\downarrow}^{\dagger} c_{2\downarrow} c_{2\uparrow}^{\dagger} c_{1\uparrow}\rangle$$
$$+ \langle c_{1\uparrow}^{\dagger} c_{2\uparrow}\rangle - \langle n_{1\downarrow} c_{1\uparrow}^{\dagger} c_{2\uparrow}\rangle + \langle n_{2\downarrow} c_{1\uparrow}^{\dagger} c_{2\uparrow}\rangle) \bar{f}_{-}$$

$$+ (\langle n_{1\uparrow}\rangle - \langle n_{1\uparrow} n_{2\uparrow}\rangle + \langle c_{1\downarrow}^{\dagger} c_{2\downarrow} c_{1\uparrow}^{\dagger} c_{2\uparrow}\rangle + \langle c_{1\downarrow}^{\dagger} c_{2\downarrow} c_{2\uparrow}^{\dagger} c_{1\uparrow}\rangle$$
$$+ \langle c_{1\uparrow}^{\dagger} c_{2\uparrow}\rangle - \langle n_{1\downarrow} c_{1\uparrow}^{\dagger} c_{2\uparrow}\rangle + \langle n_{2\downarrow} c_{1\uparrow}^{\dagger} c_{2\uparrow}\rangle)(a_{+} f_{1+} + a_{-} f_{2+})$$

$$- (\langle n_{1\uparrow}\rangle - \langle n_{1\uparrow} n_{2\uparrow}\rangle + \langle c_{1\downarrow}^{\dagger} c_{2\downarrow} c_{1\uparrow}^{\dagger} c_{2\uparrow}\rangle + \langle c_{1\downarrow}^{\dagger} c_{2\downarrow} c_{2\uparrow}^{\dagger} c_{1\uparrow}\rangle$$
$$- \langle c_{1\uparrow}^{\dagger} c_{2\uparrow}\rangle + \langle n_{1\downarrow} c_{1\uparrow}^{\dagger} c_{2\uparrow}\rangle + \langle n_{2\downarrow} c_{1\uparrow}^{\dagger} c_{2\uparrow}\rangle)(a_{-} f_{1-} + a_{+} f_{2-})$$

where
$$f_{\pm} = f(\epsilon \pm t) , \quad \bar{f}_{\pm} = f(\epsilon + U \pm t) ,$$

$$f_{1\pm} = f(\lambda_{1\pm}) , \quad f_{2\pm} = f(\lambda_{2\pm})$$

Similarly, the dispersion relation arising from $\langle n_{i,\sigma} \rangle = \langle c_{i,\sigma}^{\dagger} c_{i,\sigma} \rangle$ is given by:

$$.4\langle n_{1\uparrow} \rangle = \Big(2 - 3\langle n_{1\uparrow} \rangle + \langle n_{1\uparrow} n_{2\uparrow} \rangle - \langle c_{1\downarrow}^{\dagger} c_{2\downarrow} c_{1\uparrow}^{\dagger} c_{2\uparrow} \rangle - \langle c_{1\downarrow}^{\dagger} c_{2\downarrow} c_{2\uparrow}^{\dagger} c_{1\uparrow} \rangle $$
$$- \langle c_{1\uparrow}^{\dagger} c_{2\uparrow} \rangle + \langle n_{1\downarrow} c_{1\uparrow}^{\dagger} c_{2\uparrow} \rangle + \langle n_{2\downarrow} c_{1\uparrow}^{\dagger} c_{2\uparrow} \rangle \Big) f_{+}$$

$$+ \Big(2 - 3\langle n_{1\uparrow} \rangle + \langle n_{1\uparrow} n_{2\uparrow} \rangle - \langle c_{1\downarrow}^{\dagger} c_{2\downarrow} c_{1\uparrow}^{\dagger} c_{2\uparrow} \rangle - \langle c_{1\downarrow}^{\dagger} c_{2\downarrow} c_{2\uparrow}^{\dagger} c_{1\uparrow} \rangle $$
$$+ \langle c_{1\uparrow}^{\dagger} c_{2\uparrow} \rangle - \langle n_{1\downarrow} c_{1\uparrow}^{\dagger} c_{2\uparrow} \rangle - \langle n_{2\downarrow} c_{1\uparrow}^{\dagger} c_{2\uparrow} \rangle \Big) f_{-}$$

$$+ \Big(\langle n_{1\uparrow} \rangle + \langle n_{1\uparrow} n_{2\uparrow} \rangle - \langle c_{1\downarrow}^{\dagger} c_{2\downarrow} c_{1\uparrow}^{\dagger} c_{2\uparrow} \rangle - \langle c_{1\downarrow}^{\dagger} c_{2\downarrow} c_{2\uparrow}^{\dagger} c_{1\uparrow} \rangle $$
$$- \langle c_{1\uparrow}^{\dagger} c_{2\uparrow} \rangle + \langle n_{1\downarrow} c_{1\uparrow}^{\dagger} c_{2\uparrow} \rangle + \langle n_{2\downarrow} c_{1\uparrow}^{\dagger} c_{2\uparrow} \rangle \Big) \overline{f}_{+}$$

$$+ \Big(\langle n_{1\uparrow} \rangle + \langle n_{1\uparrow} n_{2\uparrow} \rangle - \langle c_{1\downarrow}^{\dagger} c_{2\downarrow} c_{1\uparrow}^{\dagger} c_{2\uparrow} \rangle - \langle c_{1\downarrow}^{\dagger} c_{2\downarrow} c_{2\uparrow}^{\dagger} c_{1\uparrow} \rangle $$
$$+ \langle c_{1\uparrow}^{\dagger} c_{2\uparrow} \rangle - \langle n_{1\downarrow} c_{1\uparrow}^{\dagger} c_{2\uparrow} \rangle - \langle n_{2\downarrow} c_{1\uparrow}^{\dagger} c_{2\uparrow} \rangle \Big) \overline{f}_{-}$$

$$+ \Big(\langle n_{1\uparrow} \rangle - \langle n_{1\uparrow} n_{2\uparrow} \rangle + \langle c_{1\downarrow}^{\dagger} c_{2\downarrow} c_{1\uparrow}^{\dagger} c_{2\uparrow} \rangle - \langle c_{1\downarrow}^{\dagger} c_{2\downarrow} c_{2\uparrow}^{\dagger} c_{1\uparrow} \rangle $$
$$+ \langle c_{1\uparrow}^{\dagger} c_{2\uparrow} \rangle - \langle n_{1\downarrow} c_{1\uparrow}^{\dagger} c_{2\uparrow} \rangle - \langle n_{2\downarrow} c_{1\uparrow}^{\dagger} c_{2\uparrow} \rangle \Big)$$
$$\Big[(1 + 2\alpha_1 \alpha_2) f_{1+} + (1 - 2\alpha_1 \alpha_2) f_{2+} \Big]$$

$$+ \Big(\langle n_{1\uparrow} \rangle - \langle n_{1\uparrow} n_{2\uparrow} \rangle + \langle c_{1\downarrow}^{\dagger} c_{2\downarrow} c_{1\uparrow}^{\dagger} c_{2\uparrow} \rangle + \langle c_{1\downarrow}^{\dagger} c_{2\downarrow} c_{2\uparrow}^{\dagger} c_{1\uparrow} \rangle $$
$$- \langle c_{1\uparrow}^{\dagger} c_{2\uparrow} \rangle + \langle n_{1\uparrow} c_{1\uparrow}^{\dagger} c_{2\uparrow} \rangle + \langle n_{2\downarrow} c_{1\uparrow}^{\dagger} c_{2\uparrow} \rangle \Big)$$
$$\Big[(1 - 2\alpha_1 \alpha_2) f_{1-} + (1 + 2\alpha_1 \alpha_2) f_{2-} \Big]$$

From the orthogonality condition $\left(\left(\Psi^1_{2\downarrow}, \Psi^2_{2\uparrow}\right)\right) = 0$, an additional

relation is obtained:

$$\alpha_1 \alpha_2 \left(\langle n_{1\uparrow} n_{1\downarrow} \rangle - \langle n_{1\uparrow} n_{2\downarrow} \rangle + \langle c^\dagger_{1\downarrow} c_{2\downarrow} c^\dagger_{1\uparrow} c_{2\uparrow} \rangle - \langle c^\dagger_{1\downarrow} c_{2\downarrow} c^\dagger_{2\uparrow} c_{1\uparrow} \rangle \right)$$

$$+ \left(\alpha^2_2 - \alpha^2_1 \right) \left(\langle n_{1\downarrow} c^\dagger_{1\uparrow} c_{2\uparrow} \rangle + \langle n_{2\downarrow} c^\dagger_{1\uparrow} c_{2\uparrow} \rangle \right.$$

$$\left. - 2 \langle n_{1\downarrow} n_{2\downarrow} c^\dagger_{1\uparrow} c_{2\uparrow} \rangle \right)$$

$$= \langle n_{1\downarrow} c^\dagger_{1\uparrow} c_{2\uparrow} \rangle - \langle n_{2\downarrow} c^\dagger_{1\uparrow} c_{2\uparrow} \rangle$$

JUDD OPERATOR METHODS IN SUPERSPACE: APPLICATION TO THE THERMAL SINGLE-PARTICLE GREEN FUNCTION FOR THE HUBBARD DIMER

by

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(ABSTRACT)

The Fourier transforms of the thermal two-time single-particle Green functions may be expressed as matrix elements of the resolvent of the Liouville operator, in an abstract Hilbert space. This abstract Hilbert space (the "superspace") contains elements f, g, etc. which are products of an odd number of fermion creation and/or annihilation operators. These operators may also be expressed as linear combinations of a set of stepping operators ϕ = fIg, where I is the projection operator for the vacuum in the ordinary Fock space. The Judd operators are stepping operators which step between many-particle states which usually differ in particle number. In the calculation of the single-particle Green function, only those single-particle Judd operators which step between states differing by one electron are relevant. The Judd operators obey a Lie algebra analogous to the angular momentum stepping operators $L_{\pm}$. The single-site and two-site Hubbard model for arvitrary electron density are solved exactly using the Judd operator formalism. The correlation functions are evaluated as functions of chemical potential, temperature and t/U, where t is the hopping energy and U is the intasite Coulomb energy.