STUDIES IN RELAXATION

by

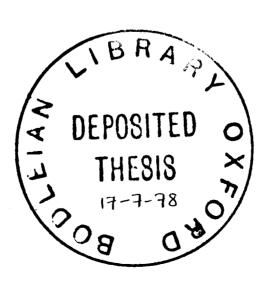Savas Hadjipavlou

A thesis submitted for the Degree Doctor of Philosophy

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ABSTRACT

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A thesis submitted for the degree of Doctor of Philosophy by

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This work concerns itself with the exact study of the dynamical properties of two model systems. After a brief summary of theory and concepts previous work is discussed, and this provides the motivation for the formulation of the first model. This quantum mechanical lattice model and some of its equilibrium properties are described in Chapter II. The dynamical problem to be studied is formulated in Chapter III; this is essentially the study of the time evolution (generated by the Hamiltonian) of a finite system at temperature T_1 coupled to an infinite copy of itself at a temperature T_2 and acting as a heat bath for the system. The problem is solved for the special case, when the coupling as scaled by the parameter γ, takes the value $\gamma = 1$.

The general case for arbitrary γ values is treated in Chapter IV. It is shown that the system approaches the equilibrium state of the heat bath in a non-exponential manner, provided the spectrum of the Hamiltonian is continuous and does not have a discrete part. This result is in complete accord with the findings of other work summarised in Chapter I. The mixing properties of the model and behaviour of the relaxation rate in the weak coupling limit are studied in Chapter V. The model is shown to fail to behave as a calorimeter and in view of this result the relevance of the concept of mixing to irreversible behaviour is discussed. The main conclusions and results for the model are summarised at the end of Chapter V.

The second model discussed, was first introduced by R.J. Glauber to study the dynamics of the Ising chain. The main feature here is that the time evolution is defined through a Master equation, and the associated stochastic operator. It is shown in Chapter VI that exploiting fully the free fermion character of the stochastic operator for the Glauber model, it is possible to provide a simple method to the study of the dynamics of the Ising Chain.

CHAPTER I. INTRODUCTION

One of the important tasks of Statistical Mechanics is to provide explanations to the range of phenomena exhibited by physical systems undergoing large scale changes with time. This task has been hampered with very difficult problems, largely of a mathematical nature; the extreme complexity of interacting many body systems has meant that any attempt at rigorous analysis of their dynamical properties is doomed to failure. Thus, inspite of over a century of study, the general principles of non-equilibrium statistical mechanics are not clearly understood, and remain in largest measure unformulated. This situation may be compared with the statistical study of systems at equilibrium. Here, although the problems are still great, they are at least well formulated.

Faced with formidable difficulties in obtaining a clear understanding of the time dependent behaviour in real systems, theorists have devoted a great deal of effort to devise and study, simple model systems. The main objectives in these studies are that, (i) the models should permit exact treatment, (ii) still show some resemblence to real systems. The understanding and deeper insight offered by the exact solutions is intended to compensate for the simplicity of the models.

Two types of model systems have been studied: The first, truly mechanical models, are based on Liouville's equation. An initial probability is introduced, this probability being then allowed to evolve in time, by Liouville's equation. The uncertainty about the initial state introduced in this way, is sufficient to bring irreversible behaviour into the problem. The major portion of this work will be concerned with the analysis of the time evolution, for just such a model described in Chapter II. The second class of model systems extensively studied, are non-mechanical in character, with the important characteristic that probability is introduced into the problem at all times. Traditional theory of non-equilibrium processes centres around the Boltzmann and Master equations both of which

make this kind of statistical assumption. The time evolution in these cases is clearly not deterministic in the mechanical sense. We consider only a particular example of such a model. The relevant introductory details, and theory may be found in Chapter VI.

In this Chapter, sections 1 and 2 describe some of the concepts used to describe the properties of the time evolution in classical systems and the corresponding ideas for quantum systems. This provides the relevant background for discussion in section 3, of the results obtained by exact study of simple mechanical systems, which in turn motivates our work in Chapters II to V. Comparison of our results with earlier work is made at the end of Chapter V.

1. Ergodicity, Mixing, and Decay of Correlation functions [1]

The dynamics of classical Hamiltonian systems are described in the phase space of conjugate canonical variables (p,q), Γ. The state of a classical system is represented by a point in this space

$$x = (\underline{p},\underline{q}) \in \Gamma \tag{1.1}$$

$$\underline{p} = (p_1 \cdots p_{3N}); \quad \underline{q} = (q_1 \cdots q_{3N})$$

where we have taken the system to consist of N identical particles, interacting via a potential V, in a bounded domain of configuration space Ω. The Hamiltonian is

$$H(\Omega) = \sum_i \frac{p_i^2}{2m} + V(q_1 \cdots q_{3N}) \tag{1.2}$$

where $\underline{q} \epsilon \Omega$ and $v(q) > - k; \quad k < \infty$.

The time independent Hamiltonian (1.2) generates the time evolution of the system, though the canonical equations of motion

$$\dot{q}_i = \frac{\partial H}{\partial p_i}; \quad \dot{p}_i = - \frac{\partial H}{\partial q_i} \tag{1.3}$$

Equations (1.3) describe the motion of the representative point $\underline{x}(t)$ in the phase space Γ. In the case of conservative systems the flow will be restricted to a 'surface' in Γ, S_E, given by

$$H(\Omega) \;=\; E \tag{1.4}$$

The time evolution of any function $f(\underline{x})$ is given by

$$\frac{df}{dt} \;=\; [f,H]_{P.B} \;=\; i\hat{L}f \tag{1.5}$$

where $\hat{L}$ is the Liouville operator corresponding to the usual Poisson bracket

$$\hat{L} \;=\; i \sum_j \left[\frac{\partial H}{\partial q_j} \frac{\partial}{\partial p_j} - \frac{\partial H}{\partial p_j} \frac{\partial}{\partial q_j} \right] \tag{1.6}$$

and that of an ensemble density $\rho(x,t)$ by

$$\frac{\partial \rho(x,t)}{\partial t} \;=\; -\,i\hat{L}\rho \tag{1.7}$$

Every non-negative $\rho(x,t)$ defines a measure μ on Γ, the measure of a set A being taken to be

$$\mu(A,t) \;=\; \int_A \rho(x,t)\ dx \tag{1.8}$$

with $\mu(\Gamma,t) = 1$. Of importance to statistical mechanics are the time independent measures

$$\rho(x,t) \;=\; \rho_o(x) \tag{1.9}$$

examples of which are the familiar micro-canonical and canonical ensembles,

$$d\mu_o \;=\; \omega^{-1}(\varepsilon)\ \frac{d\sigma}{|\mathrm{grad.}\ H(\underline{x})|} \qquad x\varepsilon S_E$$

$$=\; 0 \text{ otherwise}$$

$$\omega(\varepsilon) = \int_{S_E} \frac{d\sigma}{|\text{grad. } H(\underline{x})|} \qquad (1.10)$$

$d\sigma$ = element of 'surface' area

$$d\mu_o = Z^{-1} e^{-\beta H(\underline{x})} dx$$

$$Z = \int_0^\infty \omega(E) e^{-\beta E} dE \qquad (1.11)$$

We can now give the definitions for ergodic and mixing flows as generated by the Hamiltonian $H(\Omega)$. We restrict these to the case of conservative systems, that is the flow is on S_E, and use the microcanonical ensemble (1.10) as our time invariant measure.

Definition 1. (Birkoff, [5])

A system is said to be ergodic on an energy surface S_E if and only if

$$\lim_{T\to\infty} \frac{1}{T} \int_0^T f(x(t)) dt = \int_{S_E} f(\underline{x}) d\mu_o \qquad (1.12)$$

for all $f(\underline{x})$ such that $\int d\mu_o |f(\underline{x})| < \infty$. This condition is allowed to fail for sets whose measure w.r.t. $d\mu_o$ is zero.

Definition 2. (Hopf [5])

A Hamiltonian flow on S_E is called mixing if and only if

$$\lim_{t\to\infty} \mu_o(A_t \cap B) = \mu_o(A) \mu_o(B) \qquad (1.13)$$

where $\mu_o(S_E) = 1$, for all A, B, $\subset S_E$ s.t $\mu_o(A) > 0$ and A_t is the set A is mapped into, after time t.

Definition 1 implies that the trajectory of the point x(t), will sample all regions of the available surface S_E, and so consequently that

it is permissible to replace the time average, by the integral over S_E.
Clearly if it were possible to partition the energy surface S_E into two
sets of measure greater than zero, so that the trajectory was confined to
any one of them, the system would fail to be ergodic. The definition says
nothing about the way the trajectory samples the surface S_E, and in
principle this can be very ordered, or disordered [6].

A stronger condition on the flow generated by the Hamiltonian H, is
that it be mixing. This notion was first invented by Gibbs who thought
that the motion on S_E could be likened to the stirring of two incompressible
miscible fluids to produce a uniform whole. Definition 2 is a mathematical
description of this idea. The proportion of systems originally in A_t,
and which are also located in some fixed set B (ie $A_t \cap B$) in the limit
of $t \to \infty$ approaches the ratio of the volume of B to that of S_E. This means
that the set A_t becomes uniformly spread on S_E.

Mixing implies a strong instability property of the equations of
motion, that is, an imprecise measurement of the initial state $\underline{x}(o)$ gives
no useful information as to its behaviour at large times. It thus represents
a more turbulent flow on S_E than ergodicity, and we can show that mixing
implies ergodicity. Suppose that $A \subset S_E$ is an invariant set. If such a set
existed, then the system would not be ergodic. We show that $\mu(A) = 0$, or 1

(i) $A_t \cap A = A$ by invariance

(ii) $\mu(A_t \cap A) = \mu(A) \mu(A)$ by mixing   (1.14)

$\Rightarrow \mu(A) = 0$ or 1.

We can connect the motion of mixing, directly with the formalism of
statistical mechanics by means of correlation functions. This can be done
through the auxiliary formalism introduced by Koopman [7], who observed
that for square integrable functions f, g defined on S_E, and with respect
to the invariant measure $d\mu_o$ form a Hilbert space with scalar product

$$<f,g> = \int_{S_E} f^*(\underline{x}) g(\underline{x}) d\mu_o \qquad (1.15)$$

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We then have

Theorem 1.1 [8]

A system is mixing if and only if

$$<f(t)g> \xrightarrow[\quad\quad]{t \to \infty} <f><g> \tag{1.16}$$

where from (1.5)

$$f(t) = e^{it\hat{L}} f(x) = f(\mathcal{X}(t)) \tag{1.17}$$

and

$$<f> = \int_{S_E} f(x) d\mu_o$$

The operator $U_t = e^{it\hat{L}}$ is unitary (the flow is measure preserving) and forms a continuous one parameter group of automorphisms on the algebra of dynamical functions $f(p,q)$, the Liouville operator being self adjoint,

$$\hat{L}^\dagger = \hat{L} \tag{1.18}$$

This formulation of mixing, reflects the unstable character of the equations of motion, in that for large times, systems which might have.been close together are no longer correlated.

The ergodic and mixing properties of a flow can also be characterised in terms of the spectral properties of the Liouville operator $\hat{L}$. In general $\hat{L}$ will have a discrete and continuous part to its spectrum, the following characterisation has been found [9].

(i) The flow is ergodic if and only if constant functions are the only invariant functions, ie if zero is a simple eigenvalue of $\hat{L}$. This corresponds to our inability to partition S_E into two invariant sets, when no other constants of the motion, other than the energy exist. Constant functions are always eigenfunctions of $\hat{L}$ with eigenvalue zero, since U_t leaves such functions invariant.

(ii) When the flow is mixing, $\hat{L}$ has a simple eigenvalue 0, and the rest of the spectrum is continuous. The converse is not quite true. A system has the weak mixing property if and only if zero is the only member of the discrete part of the spectrum of $\hat{L}$ and it is non-degenerate. Apart from this value the spectrum of a weakly mixing system is continuous. A system is weakly mixing if

$$\lim_{T \to \infty} \frac{1}{T} \int_0^T \left| \mu(A_t \cap B) - \mu(A) \, \mu(B) \right| \, dt = 0 \qquad (1.19)$$

for all sets A, B, $\subset S_E$. This property is intermediate between those of ergodicity and mixing, and indicates that the spreading of A_t through the energy surface may become non-uniform at a set of isolated instants in time.

By making stronger assumptions about the continuity of the spectrum of $\hat{L}$, namely that $\hat{L}$ has a homogeneous Lebesgue spectrum [3] we can prove the mixing property. This means that every real number λ, apart from zero, lies in the spectrum of $\hat{L}$, has the same multiplicity, and the spectral weight is $d\lambda$. We thus have a hierarchy of properties that characterise the flow as being more and more irreversible.

H.L. spectrum => mixing => weak mixing => ergodic   (1.20)

There are some features about classical systems which must be stressed. The first is, that it is not necessary to go to the infinite volume, thermodynamic limit in order that we obtain decay of the correlation functions. The result of Sinai [10], that a system consisting of a finite number N (N $\geq$ 2) of hard spheres is a mixing system indicates two things.

(i) Finite classical systems can and do have purely continuous spectra.

(ii) Mixing ensures that the Poincaré recurrence times for the two systems which are initially close together are wildly different, so that

the sets A_t described earlier become uniformly distributed on S_E.

2. Quantum Systems

The situation for quantum systems is not too different to that of classical systems. The exception is that for a system confined to a bounded domain Ω, and with reasonably physical interactions, its Hamiltonian has a discrete spectrum. This means that the expected value of any measurement will be an almost periodic function of time. Although for macroscopic systems the level spacing will be extremely fine, it is necessary to consider infinite systems in order that we obtain mathematically sharp results.

It is well known [11] that states of a finite quantum system are represented by density operators ρ_Ω, the expectation value of any observable A being given by

$$<A>_{\rho\Omega} \quad = \quad Tr(\rho_\Omega A) \tag{1.21}$$

The time evolution generated by the Hamiltonian $H(\Omega)$ takes the form (Heisenberg picture)

$$A_\Omega(t) \quad = \quad e^{iH(\Omega)t} A(o) e^{-iH(\Omega)t} \tag{1.22}$$

We construct the states of an infinite system [12] by first evaluating (1.21) or (1.22) for a finite system confined in Ω, and then consider the limit $\Omega \to \infty$.

$$<A>_\rho \quad = \quad \underset{\Omega\to\infty}{Lim} \; <A>_{\rho\Omega}$$

$$\tag{1.23}$$

$$<A(t)>_\rho \quad = \quad \underset{\Omega\to\infty}{Lim} \; <A_\Omega(t)>_{\rho\Omega}$$

Thus states for the infinite system are constructed as limits of finite-volume states.

Primarily we would like to show that in the infinite system, starting

in a non-equilibrium state represented by the density operator π, under the time evolution generated by $H(\Omega)$, we obtain an equilibrium state ρ.

$$\lim_{t\to\infty} <A(t)>_\pi = <A>_\rho \qquad (1.24)$$

Secondly what does the mixing property tell us about (1.24)? By analogy of Theorem 1.1 we can define a mixing system to be

$$\lim_{t\to\infty} <A(t) \; B(0)> = <A><B> \qquad (1.25)$$

where ρ is an equilibrium state, with A, and B operators representing all local measurements on the infinite system. This is clearly a decay in the correlation between the observables A(t), and B, when in the limit $t \to \infty$ they become statistically independent.

It has been shown [12] that given a non-equilibrium state π, then the time average of the state π approaches the equilibrium state ρ provided (1.25) is true, that is

$$\lim_{T\to\infty} \frac{1}{2T} \int_{-T}^{T} <A(t)>_\pi \cdot dt = <A>_\rho \qquad (1.26)$$

This result is of the type, ergodicity is implied by mixing. In this work we shall be concerned with establishing the validity of (1.24) and (1.25), and in particular, what happens when we consider global rather than local deviations from equilibrium for a particular model, to be introduced in Chapter II. In the next section we briefly summarise some of the results established for some model systems and their relevance to the theoretical framework already discussed.

3. Model Systems

Due to insurmountable difficulties in deciding whether a Hamiltonian

for a realistic model satisfies the properties outlined earlier, attention has been turned to simple harmonic systems. The simplicity of these models allows us to study exactly their dynamics, and therefore investigate the validity of equations (1.24) and (1.25).

Mazur and Montrol [13] studied the behaviour of the velocity auto-correlation function in a harmonic crystal, of N particles. They found that in the limit $N \to \infty$, and for large times the velocity autocorrelation behaved as $t^{-d/2}$, with d the dimensionality of the crystal lattice.

$$<v_j(t) \cdot v_j(o)> = \lim_{N \to \infty} <v_j(t) \, v_j(o)>_N \sim t^{-d/2} \qquad (1.27)$$

The limit $N \to \infty$ is essential in that it produces a continuum of vibrational modes, and the essential feature in the decay of the auto-correlation function appears to be the absence of localised modes in this limit. In view of our earlier discussion this would "correspond" to the Liouville operator $\hat{L}$ not having any discrete eigenvalues in this limit.

The effect of an isolated mode in determining the properties of local phase functions has been exhibited in the work of Cuckier and Mazur [14], who study the kinetic energy of an impurity of mass M, embedded in an equal mass chain (m) of harmonic oscillators. They find that the kinetic energy is ergodic/non-ergodic as $\mu = (\frac{M}{m}) \geq 1$, or < 1 and attribute this behaviour to the absence/presence of an isolated mode in the frequency spectrum of the Hamiltonian in the limit $N \to \infty$.

In quantum systems the dynamics of the X-Y model [15] have been extensively studied. It has proved possible to obtain many of its equilibrium [16] and dynamical properties [17,18] exactly for the case where interactions are restricted to nearest neighbours. For a one dimensional lattice the Hamiltonian is of the form

$$H(\Omega) = \sum_{(n \epsilon \Omega)} \{(1 + \gamma) \, \sigma_n^x \sigma_{n+1}^x + (1 - \gamma) \, \sigma_n^y \sigma_{n+1}^y + h_n \sigma_n^z\}$$

$$(1.28)$$

where $\sigma_n{}^x$, $\sigma_n{}^y$, $\sigma_n{}^z$ are the Pauli spin operators, h_n and γ are external field, and anisotropy parameters respectively.

Niemeijer [17] has studied the time dependent correlations functions of the z components of spins at lattice sites n, and n+R, ie

$$<\sigma_n{}^z\sigma_{n+R}{}^z(t)>_\rho = \text{Tr}(\rho \; \sigma_n{}^z \; e^{iH(\Omega)t} \; \sigma_{n+R}{}^z \; e^{-iH(\Omega)t}) \qquad (1.29)$$

where ρ is the equilibrium, Gibbs density state. It was found that

$$\left[\lim_{|\Omega| \to \infty} <\sigma_n{}^z\sigma_{n+R}{}^z(t)> \right] \underset{\sim}{\overset{t \to \infty}{}} <\sigma_n{}^z><\sigma_{n+R}{}^z> + O(t^{-1}) \qquad (1.30)$$

a result which can easily be related to (1.25). The validity of (1.24) was also studied for the total magnetisation, where the equilibrium and non-equilibrium states are obtained by a variation of the external field parameter (h_n = h for all n in this case). It was found that (1.24) was not satisfied, and this was attributed to the global character of the perturbation.

A similar study by Abraham et al [19], but with the perturbation now localised to a single spin yielded different results. These authors again studied (1.24) for a single spin embedded in the chain, but subjected two types of perturbation

(i) h_n = 0 except for n = j $t \leq 0$

        h_n = 0 for all n $t > 0$

(ii) h_n = 0 for all n $t \leq 0$

        h_n = 0 except for n = j $t > 0$

It was found that $<\sigma_j{}^z(t)>_\pi$ satisfied (1.24) for case (i) but not for (ii). This difference was due to the presence of an isolated eigenvalue in the spectrum of the Hamiltonian generating the time evolution (in the limit $\Omega \to \infty$).

Two general features of these models are

(i)   It is necessary to consider infinite systems in order that we obtain continuous spectra.

(ii)   Local functions have mixing properties, these being generally inhibited by the presence of isolated eigenvalues in the frequency spectrum of the Hamiltonian which generates the time evolution.

The work carried out in these models considered the system to be observed as being a single spin or single particle.   It would be of interest to know the behaviour of the interacting system as a function of size, and how this is related to the validity of equations (1.24) and (1.25).   To this end we study some aspects of this problem by examining the thermal relaxation properties of a finite system in interaction with an infinitely large copy of itself which serves as a heat bath.   The flowchart (Fig. 1.1) indicates the contents of the major sections in the Chapters II to V and their inter-relations.

Figure 1.1

II

(i)   Introduction of lattice model, and definition of Hamiltonian.

(ii) Diagonalise Hamiltonian and obtain equilibrium state for particle density at a lattice site.

III

(i)   The equations of motion for a system coupled to a heat bath via the scaled interaction $\gamma H'$ are set up, and solved for the special case $\gamma = 1$.

Discussion of the resulting equation.

(ii) The limit $|\Omega_B| \to \infty$ is obtained. This corresponds to taking the heat bath to be of infinite extent.

(iii) Discussion of the time dependence, and approach to the equilibrium state of the heat bath.

IV

(i)   The Hamiltonian for arbitrary γ values is diagonalised and the new γ-dependent unitary transformations obtained.

(ii) The equations of motion for this general case are described.

(iii) The spectral properties of the Hamiltonian for arbitrary γ are discussed in the limit $|\Omega_B| \to \infty$. The same limit is obtained for the equations of motion.

(iv) Discussion of the time evolution, and its behaviour with respect to the spectral properties of the Hamiltonian.

V

(i)   Mixing properties of the Hamiltonian are examined.

(ii) Time dependence in the weak coupling limit is obtained. Dependence of the relaxation rate on the size of the system is shown.

(iii) Failure of the model to show calorimetric behaviour is illustrated and inadequacy of mixing concept discussed.

(iv) Conclusions and Discussion.

CHAPTER II. THE MODEL

In this chapter a quantum mechanical many body model is introduced; this is to be used in subsequent chapters to study the time dependent properties of interacting systems. Section 1 describes this model and in section 2 we study some of its equilibrium properties.

1. The Model

We represent the spatial extension of a physical system by a cylindrical lattice Ω (fig. 1) characterised by its length and circumference of N and M lattice points respectively. The lattice points are labelled by the coordinates (n,m) so that
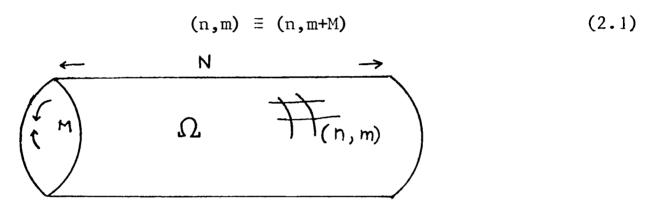
$$(n,m) \equiv (n,m+M) \qquad (2.1)$$

Figure 1. The lattice Ω.

A physical system is defined by attributing to it a Hamiltonian $H(\Omega)$ and we choose H (Ω) to be composed of the fermion lattice operators $f^{\dagger}_{nm}$, and f_{nm}

$$H(\Omega) = \frac{1}{2} \sum_{(n,m)\varepsilon\Omega} (f^{\dagger}_{n+1,m} f_{nm} + f^{\dagger}_{n,m+1} f_{nm} + h.c) \qquad (2.2)$$

where only nearest neighbour terms are allowed. The lattice operators obey the anticommutation rules

$$[f^{\dagger}_{nm}, f_{rs}]_{+} = \delta_{nr}\delta_{ms}$$

$$[f^{\dagger}_{nm}, f^{\dagger}_{rs}]_{+} = [f_{nm}, f_{rs}]_{+} = 0 \qquad (2.3)$$

and act on points with coordinates (n,m). The operator $f^{\dagger}_{nm}$ creates a particle at (n,m) and similarly f_{nm} annihilates a particle at (n,m). Due to the anticommutation rules (2.3) an exclusion principle applies, so that only zero, or one particles can occupy a lattice site. The Hamiltonian

$H(\Omega)$ can thus be interpreted as representing the motion of such particles on the lattice Ω; the effect of terms of the type $f^{\dagger}_{nm}f_{rs}$ being to annihilate a particle at (r,s) and create one at (n,m).

2. Equilibrium Properties

The state of a quantum system in thermodynamic equilibrium at a temperature T is represented by the density operator ρ

$$\rho = \frac{e^{-\beta H(\Omega)}}{Z(\beta)} \qquad (2.4)$$

$H(\Omega)$ is the Hamiltonian of the quantum system, $\beta = (KT)^{-1}$ with K the Boltzmann constant. The quantity $Z(\beta)$ is known as the partition function, and normalises ρ

$$Z(\beta) = \text{Tr } e^{-\beta H(\Omega)}. \qquad (2.5)$$

The expectation value of any observable A of the system is given by the trace

$$\langle A \rangle_{\beta} = \text{Tr } (\rho A) \qquad (2.6)$$

and in particular we shall be interested in the properties of $\langle f^{\dagger}_{nm}f_{nm} \rangle_{\beta}$ which is the average number of particles of (n,m) when the system is at a temperature T, that is we want to evaluate

$$\langle f^{\dagger}_{nm}f_{nm} \rangle_{\beta} = \frac{\text{Tr}(f^{\dagger}_{nm}f_{nm} \, e^{-\beta H(\Omega)})}{Z(\beta)} \qquad (2.7)$$

As the trace operation is invariant of the representation in which it is carried out, (2.7) is best evaluated in the representation where $H(\Omega)$ is diagonal.

$$H(\Omega) = \sum_{(q,1)} \varepsilon_{q1} \sigma^{\dagger}_{q1} \sigma_{q1} \qquad (2.8)$$

That is we seek new fermion operators $\sigma^{\dagger}_{q1}$, related to $f^{\dagger}_{nm}$ via a unitary transformation so that $H(\Omega)$ takes the form (2.8). This can be achieved in two steps: firstly motivated by the cylindrical symmetry of the lattice we introduce the new fermion operators $F^{\dagger}_{n1}$ as the spatial Fourier

transform of the $f^\dagger_{nm}$

$$F^\dagger_{nl} = M^{-\frac{1}{2}} \sum_{m=1}^{M} e^{im\theta_1} f^\dagger_{nm} \qquad (2.9)$$

This transformation diagonalises $H(\Omega)$ with respect to the coordinate m, and imposing the cyclic boundary condition (2.1) we obtain for θ_1

$$\theta_1 = \frac{21\pi}{M} \quad 1 \leq 1 \leq M \qquad (2.10)$$

In this intermediate representation $H(\Omega)$ is

$$H(\Omega) = \frac{1}{2} \sum_{n=1}^{N} \sum_{l=1}^{M} (F_{n+1,1}F_{n,1} + 2\cos\theta_1 F^\dagger_{nl}F_{nl} + F^\dagger_{n,1}F_{n+1,1}) \qquad (2.11)$$

We can now complete the diagonalisation by defining a second transformation which brings (2.11) into diagonal form with respect to the coordinate n.

$$\sigma^\dagger_{ql} = \left(\frac{2}{N+1}\right)^{\frac{1}{2}} \sum_{n} \sin.n\phi_q F^\dagger_{nl} \qquad (2.12)$$

where with periodic boundary conditions we obtain

$$\phi_q = \frac{q\pi}{N+1} \quad 1 \leq q \leq N \qquad (2.13)$$

$H(\Omega)$ is now in the form (2.8) where the eigenvalues ε_{ql} are

$$\varepsilon_{ql} = (\cos\phi_q + \cos\theta_1) \qquad (2.14)$$

and $\sigma^\dagger_{ql}$ are the new fermion operators defined in (2.12).

Before proceeding to calculate (2.7) we can make the following important observations.

(i) Owing to the fact that we have a finite quantum system confined to a finite domain, the spectrum of $H(\Omega)$ as given by ε_{ql} is entirely discrete.

(ii) The separability of the motion in the two directions n and m allowed the application of two different transformations each of which

diagonalised $H(\Omega)$ with respect to n, or m. As a consequence of this the eigenvalues ε_{q1} are a sum of the eigenvalues corresponding to each direction of motion.

To calculate equations (2.5) and (2.7) we observe that the new fermion operators act on the occupation states $|N_{q1}>$ of the various quantum states characterised by (q,1). The occupation state of the fermion system, $|N>$, defined as the product space spanned by the occupation states for the various quantum states is

$$|N> \;=\; |N_{1,1},N_{12},\cdots N_{q1},\cdots> \;=\; \prod_{q,1} |N_{q1}> \qquad (2.15)$$

with $N_{q1} = 0$, or 1.

From (2.5) we have

$$Z(\beta) \;=\; \sum_{\substack{N_{q1}=0 \\ \text{for all } (q,1)}} <N|\; e^{-\beta H(\Omega)} |N>$$

$$= \prod_{q,1} \sum_{N_{q1}=0}^{1} <N_{q1}|e^{-\beta \varepsilon_{q1} \sigma_{q1}^{\dagger} \sigma_{q1}}|N_{q1}>$$

$$= \prod_{q,1} (1 + e^{-\beta \varepsilon_{q1}}) \qquad (2.16)$$

where equation (2.8) was used.

Equation (2.7) can be evaluated in a similar manner by first expressing $f_{nm}^{\dagger} f_{nm}$ in the $\sigma_{q1}^{\dagger}$, representation

$$f_{nm}^{\dagger} f_{nm} \;=\; \frac{2}{M(N+1)} \sum_{1,1'} \sum_{q,q'} e^{im(\theta_1 - \theta_1')} \cdot \sin n\phi_q \cdot \sin n\phi_{q'} \, \sigma_{q1}^{\dagger} \sigma_{q'1'}$$

$$(2.17)$$

Using (2.17) in (2.7) and calculating the trace we obtain for the average particle density of (n,m)

$$\langle f^\dagger_{nm} f_{nm} \rangle_\beta = \frac{2}{M(N+1)} \sum_{q,l} \frac{\sin^2 n\phi_q}{1+e^{\beta \varepsilon_{ql}}} \qquad (2.18)$$

As discussed earlier we are interested in the equilibrium state of the infinite system, that is in the thermodynamic limit $|\Omega| \to \infty$. This can be achieved by taking the limits $M, N \to \infty$ in equation (2.18). Using the definition of the Riemann integral we can replace the sums in (2.18) by corresponding integrations over θ, and ϕ

$$\lim_{|\Omega| \to \infty} \langle f^\dagger_{nm} f_{nm} \rangle_\beta = \frac{1}{2\pi^2} \int_0^{2\pi} \int_0^\pi \frac{2\sin^2 n\phi}{1+e^{\beta(\cos\theta+\cos\phi)}} d\phi . d\theta \qquad (2.19)$$

The cylindrical symmetry of the lattice ensures that $\langle f^\dagger_{nm} f_{nm} \rangle$ is translationally invariant with respect to the coordinate m, but in the limit $|\Omega| \to \infty$, and well away from the edges of the lattice we would expect this to be true for the coordinate n. The limit $n \to \infty$ in (2.19) should give the translationally invariant equilibrium state of $f^\dagger_{nm} f_{nm}$. It is easily verified that the integral in (2.19) satisfies the conditions of the Riemann-Lebesgue Lemma [20] and that this limit is

$$\lim_{n \to \infty} \langle f^\dagger_{nm} f_{nm} \rangle_\beta = \frac{1}{2\pi^2} \int_0^{2\pi} \int_0^\pi \frac{d\phi . d\theta}{1+e^{\beta(\cos\phi+\cos\theta)}} \qquad (2.20)$$

CHAPTER III. TIME EVOLUTION (SPECIAL CASE)

In this chapter we study the time dependence of the particle density ie $<f^\dagger_{nm} f_{nm}>_t$, when a system Ω_S at a temperature T_1 is in interaction with a very much larger copy of itself Ω_B, taken to be at a temperature T_2 and to act as a heat bath for Ω_S. By direct calculation of the equations of motion for $<f^\dagger_{nm} f_{nm}>_t$ (n,m) $\varepsilon \Omega_S$ we wish to ascertain whether $<f^\dagger_{nm} f_{nm}>$ approaches the equilibrium state of the heat bath and if so the rate at which this occurs.

1.   The Equations of Motion

The lattice Ω described in chapter II is divided into two parts Ω_S, and Ω_B of circumference and length M, N_s, and M, N_b respectively (see Fig. 3.1). Ω_S is taken to represent the spatial extension of the system whose
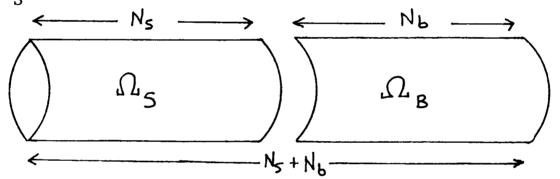
Figure 3.1

time dependent state is under study, and Ω_B that of the system which is to act as a heat bath for Ω_S.

The two regions of the lattice are initially taken to be <u>isolated</u> and the whole lattice characterised by the Hamiltonian $H_T(0)$

$$H_T(0) = H(\Omega_S) + H(\Omega_B) \tag{3.1}$$

$$\begin{matrix} H(\Omega_S) \\ or\,(\Omega_B) \end{matrix} = \frac{1}{2} \sum_{\substack{(n,m)\ \varepsilon\Omega_S \\ or\ \Omega_B}} (f^\dagger_{nm+1} f_{nm} + f^\dagger_{n+1,m} f_{nm} + h.c)$$

The equilibrium state of each isolated region of Ω is represented by the density operators

$$\rho_S = \frac{e^{-\beta_1 H(\Omega_S)}}{Z(\beta_1)} \; ; \qquad \rho_B = \frac{e^{-\beta_2 H(\Omega_B)}}{Z(\beta_2)} \qquad (3.2)$$

and because Ω_S and Ω_B are not interacting the joint state is given by the tensor product

$$\rho(0) = \rho_S \otimes \rho_B \qquad (3.3)$$

The density operator $\rho(0)$ represents the initial state of the lattice $\Omega = \Omega_S U \Omega_B$, and is the non equilibrium state π in (1.24).

Interaction between Ω_S and Ω_B is achieved by including in the total Hamiltonian for times $t > 0$ a term $\gamma H'$

$$H_\tau(t>0) = H(\Omega_S) + H(\Omega_B) + \gamma H' \qquad (3.4)$$

The interaction term H' is obtained by considering terms of the type $f^\dagger_{N_S,m} f_{N_S+1,m}$ where $N_S \varepsilon \Omega_S$, and $N_S+1 \varepsilon \Omega_B$

$$H' = \frac{1}{2} \sum_{m=1}^{M} (f^\dagger_{N_S m} f_{N_S+1,m} + h.c) \qquad (3.5)$$

The parameter γ scales the interaction such that $\gamma=0$ corresponds to the isolated systems. When $\gamma=1$, $H_\tau(t>0)$ takes the special form

$$H_\tau(t>0) = \frac{1}{2} \sum_{(m,n) \varepsilon \Omega} (f^\dagger_{n+1,m} f_{nm} + f^\dagger_{n,m+1} f_{nm} + h.c) \qquad (3.6)$$

The time evolution of $f^\dagger_{nm} f_{nm}$ $(n,m) \varepsilon \Omega_S$ is given by

$$<f^\dagger_{nm} f_{nm}>_t = Tr(\rho(0) e^{iH_\tau t} f^\dagger_{nm} f_{nm} e^{-iH_\tau t}) \qquad (3.7)$$

Equation (3.7) gives the equations of motion for an operator in the Heisenberg representation where the initial state is represented by the density operator $\rho(0)$, and H_τ is the total Hamiltonian with the inter-action term as given by (3.4).

We shall now focus our attention to the special case $\gamma=1$, and postpone a more general treatment for $\gamma>0$ until Chapter IV. As in chapter II the evaluation of the trace in (3.7) is best carried out in

representations where $H_\tau(t>0)$, and $H_\tau(t=0)$ as given by equations (3.6) and (3.1) are diagonal. The cylindrical symmetry of the lattice being preserved by the interaction term H', we transform $H_\tau(t>0)$ and $H_\tau(0)$ into the F_{nl} representation as defined by equation (2.9) to obtain

$$H_\tau(0) = \frac{1}{2} \sum_{l=1}^{M} \sum_{n\varepsilon\Omega_S} (F_{n+1,l}^\dagger F_{nl} + 2\cos\theta_1 F_{nl}^\dagger F_{nl} + F_{nl}F_{n+1,l})$$

(3.8)

$$+ \frac{1}{2} \sum_{l=1}^{M} \sum_{n\varepsilon\Omega_B} F_{n+1,l}^\dagger F_{nl} + 2\cos\theta_1 F_{nl}^\dagger F_{nl} + F_{nl}^\dagger F_{n+1,l})$$

$$H_\tau(t>0) = \frac{1}{2} \sum_{l=1}^{M} \sum_{n\varepsilon\Omega} (F_{n+1,l}^\dagger F_{nl} + 2\cos\theta_1 F_{nl}^\dagger F_{nl} + F_{nl}^\dagger F_{n+1,l})$$

(3.9)

Using the transformation defined by (2.12) and noting that $H_\tau(0)$ does not contain terms of the type $F_{N_S,l}F_{N_S+1,l}$ we define the following transformations.

$$\begin{pmatrix} \underline{\sigma} \\ \underline{n} \end{pmatrix} = \begin{pmatrix} S & 0 \\ 0 & B \end{pmatrix} \underline{F}$$

(3.10)

$$\underline{X} = T \underline{F}$$

(3.11)

where:

(i) $\underline{\sigma}$ and $\underline{n}$ are N_s and N_b dimensional vectors respectively with elements σ_{sl} and n_{bl}.

(ii) $\underline{F}$ and $\underline{X}$ are $N_s + N_b$ dimensional vectors with elements F_{nl} and X_{jl}.

(iii) The matrix in (3.10) is block diagonal, with S and B $N_s \times N_s$ and $N_b \times N_b$ dimensional matrices with matrix elements

$$S_{ns} = \left(\frac{2}{N_s+1}\right)^{\frac{1}{2}} \sin n \phi_s \qquad \phi_s = \frac{s\pi}{N_s+1}$$

(3.12)

$$1 \le s \le N_s$$

$$B_{nb} = \left(\frac{2}{N_b+1}\right)^{\frac{1}{2}} \sin (n+N_s)\phi_b \qquad \phi_b = \frac{b\pi}{N_b+1} \qquad (3.13)$$

$$1 \le b \le N_b$$

(iv) T is a $(N_s + N_b) \times (N_s + N_b)$ dimensional matrix with

$$T_{nj} = \left(\frac{2}{N_s+N_b+1}\right)^{\frac{1}{2}} \cdot \sin n\omega_j \qquad \omega_j = \frac{j\pi}{N_s+N_b+1} \qquad (3.14)$$

$$1 \le j \le N_s+N_b$$

Transformations (3.10) and (3.11) diagonalise $H_\tau(0)$ and $H_\tau(t>0)$ respectively with respect to the coordinate n. Equations (3.8) and (3.9) now take the fully diagonal forms

$$H_\tau(0) = \sum_{s,1}^{N_s,M} \varepsilon_{s1}\sigma^\dagger_{s1}\sigma_{s1} + \sum_{b,1}^{N_b,M} \varepsilon_{b,1}\eta^\dagger_{b1}\eta_{b1} \qquad (3.15)$$

$$H_\tau(t>0) = \sum_{j,1}^{N_s+N_b,M} \Lambda_{j1}X^\dagger_{j1}X_{j1} \qquad (3.16)$$

where the eigenvalues ε_{s1} ε_{b1}, and Λ_{j1} are given by

$$\varepsilon_{s1} = \cos\phi_s + \cos\theta_1$$

$$\varepsilon_{b1} \doteq \cos\phi_b + \cos\theta_1 \qquad (3.17)$$

$$\Lambda_{j1} = \cos\omega_j + \cos\theta_1$$

It is important to notice that these eigenvalues differ only through the frequencies $\cos\phi_s$, $\cos\phi_b$, $\cos\omega_j$ corresponding to interactions with respect to the coordinate n. This is a consequence of the choice of H' in (3.5). Transformations (3.10) and (3.11) can also be used to express the X_{j1} fermion operators in terms of the σ_{s1} and η_{b1} via a unitary transformation U.

$$\underline{X} = U\left(\frac{\sigma}{\eta}\right) \qquad (3.18)$$

$$U = T \begin{pmatrix} S & 0 \\ 0 & B \end{pmatrix}^{-1} \tag{3.19}$$

The matrix elements of U can be explicitly calculated from (3.19) using the definitions (3.12) to (3.14)

$$U_{js} = [(N_s+N_b+1)(N_s+1)]^{-\frac{1}{2}} \frac{\sin(N_s+1)\omega_j \cdot \sin N_s \phi_s}{\cos\omega_j - \cos\phi_s} \tag{3.20}$$

$$U_{jb} = [(N_s+N_b+1)(N_b+1)]^{-\frac{1}{2}} \frac{\sin N_s \omega_j \cdot \sin\phi_b}{\cos\omega_j - \cos\phi_b} \tag{3.21}$$

We are now in a position to calculate the trace in (3.7). By first expressing the operator $f^\dagger_{nm} f_{nm}$ in terms of the $X^\dagger_{j1}$, and X_{j1}

$$f^\dagger_{nm} f_{nm} = \frac{1}{M} \sum_{1,1'}^{M} \sum_{j,j'}^{N_s+N_b} e^{im(\theta_1 - \theta_{1'})} T_{nj} T_{nj'} X^\dagger_{j1} X_{j'1'} \tag{3.22}$$

and using the identity

$$e^{it\Lambda_{j1} X^\dagger_{j1} X_{k1}} X^\dagger_{j1} e^{-it\Lambda_{j1} X^\dagger_{j1} X_{j1}} = e^{it\Lambda_{j1}} X^\dagger_{j1} \tag{3.23}$$

We can write

$$e^{iH_\tau t} f^\dagger_{nm} f_{nm} e^{-iH_\tau t} = \tag{3.24}$$

$$\frac{1}{M} \sum_{1,1'} \sum_{j,j'} e^{im(\theta_1 - \theta_{1'})} T_{nj} T_{nj'} e^{it(\Lambda_{j1} - \Lambda_{j'1'})} X^\dagger_{j1} X_{j'1'}$$

Substituting (3.24) in (3.7) we obtain

$$\langle f^\dagger_{nm} f_{nm} \rangle_t \tag{3.25}$$

$$= \frac{1}{M} \sum_{1,1'} \sum_{j,j'} e^{im(\theta_1 - \theta_{1'})} e^{it(\Lambda_{j1} - \Lambda_{j'1'})} T_{nj} T_{nj'} \cdot T_r(\rho(0) X^\dagger_{j1} X_{j'1'})$$

To complete the calculation, we express the X_{j1} fermion operators in terms of the σ_{s1} and η_{b1} using (3.18)

$$X_{j1} = \sum_s U_{js}\sigma_{s1} + \sum_b U_{jb}\eta_{b1} \qquad (3.26)$$

We note that (3.26) implies that evaluation of the trace in (3.25) involves the calculation of the following four quantities

$$<\sigma_{s1}^\dagger \sigma_{s'1'}>; \quad <\sigma_{s1}^\dagger \eta_{b'1'}>; \quad <\eta_{b1}^\dagger \sigma_{s'1'}>; \quad <\eta_{b1}^\dagger \eta_{b'1'}> \qquad (3.27)$$

$$<\ldots> = T_r(\rho(0)\ldots)$$

Bearing in mind that the σ and η fermion operators act on the occupation states of the isolated systems Ω_S, and Ω_B, then as the two systems are uncorrelated (time $t = 0$) we have

$$<Q(S)Q(B)> = <Q(S)><Q(B)> \qquad (3.28)$$

where $Q(S)$, and $Q(B)$ act on Ω_S and Ω_B respectively. Using (3.28) we can evaluate the quantities occuring in (3.27) to obtain

$$<\sigma_{s1}^\dagger \sigma_{s'1'}> = \delta_{ss'}\delta_{11'} (1+e^{\beta_1 \varepsilon_{s1}})^{-1} \qquad (3.29)$$

$$<\sigma_{s1}^\dagger \eta_{b'1'}> = <\eta_{b1}^\dagger \sigma_{s'1'}> = 0$$

$$<\eta_{b1}^\dagger \eta_{b'1'}> = \delta_{bb'}\delta_{1'1} (1+e^{\beta_2 \varepsilon_{b1}})^{-1}$$

Equations (3.26) and (3.29) enable the complete evaluation of $<f_{nm}^\dagger f_{nm}>_t$ in (3.25) to be carried out

$$<f_{nm}^\dagger f_{nm}>_t = \frac{1}{M} \sum_{1=1}^{M} \sum_{s=1}^{N_s} <\sigma_{s1}^\dagger \sigma_{s1}>_{\beta_1} \left| \sum_j e^{itcos\omega_j} T_{nj}U_{ns} \right|^2$$

$$+ \frac{1}{M} \sum_{1=1}^{M} \sum_{b=1}^{N_b} <\eta_{b1}^\dagger \eta_{b1}>_{\beta_2} \left| \sum_j e^{itcos\omega_j} T_{nj}U_{jb} \right|^2 \qquad (3.30)$$

Equation (3.30) gives the time evolution of $f_{nm}^\dagger f_{nm}$ $(n,m)\varepsilon\Omega$. The first observation to be made about the structure of (3.30) is that it is composed of two terms each of which depends only on the temperature of

Ω_S or Ω_B. Secondly due to the special form of the spectra ε_{s1}, ε_{b1} and Λ_{j1} is given in (3.17) the time dependence is given as a sum over the j quantum states, and is independent of the 1 quantum numbers.

The coordinate n which appears in the time dependent sums could in principle be chosen to lie in either Ω_S or Ω_B, that is equation (3.30) is symmetrical with respect to Ω_S, or Ω_B, and we must choose the system we wish to observe by suitably restricting the value of n. For example $1 \leq n \leq N_S$ chooses Ω_S. An additional symmetry of this equation is that it is invariant with respect to time inversions $t \to -t$.

This equation describes the time evolution of $f^{\dagger}_{nm} f_{nm}$ when both the interacting systems Ω_S and Ω_B are of finite size. For this situation a general recurrence theorem can be stated, namely that there exists a recurrence time T_r so that the state of a system at time t is resurected at a later time $(t + T_r)$ [21]. More precisely for equation (3.30) we have; given $\varepsilon > 0$, $\exists\, T_r(\varepsilon, N_S + N_b)$ s.t.

$$|\sum_j c_j\, e^{itcos\omega_j}\, (1-e^{iT_r cos\omega_j})|^2 \leq \sum_j 2|c_j|^2\, (1-cos(T_r cos\omega_j)) < \varepsilon$$

(3.31)

From these considerations, it is clear that as long as we deal with finite systems the time behaviour will be quasi-periodic and that no approach to equilibrium can be expected. In experiments the system which is chosen to be the heat bath is several orders of magnitude larger than the system which is observed. We can introduce this distinction by letting Ω_B become infinitely large relative to the size of Ω_S. This limit, ie $|\Omega_B| \to \infty$, will distinguish between Ω_S, and Ω_B in the otherwise symmetrical equation (3.30). Moreover the recurrence time $T_r(N_S + N_b)$ which depends on the size of Ω_B now becomes infinite.

2. The Limit $|\Omega_B| \to \infty$ in Equation (3.30)

The following definitions are introduced:

(i)

$$f(\omega_j,\phi_s,t) = \frac{e^{it\cos\omega_j}\cdot\sin n\omega_j\cdot\sin(N_s+1)\omega_j}{\cos\omega_j-\cos\phi_s} \qquad (3.32)$$

(ii)

$$g(\omega_j,\phi_b,t) = \frac{e^{it\cos\omega_j}\cdot\sin n\omega_j\cdot\sin N_s\omega_j}{\cos\omega_j-\cos\phi_b} \qquad (3.33)$$

(iii)

$$I(n,t,N_s+N_b) = \frac{1}{N_s+N_b+1}\sum_j f(\omega_j,\phi_s,t) \qquad (3.34)$$

(iv)

$$S(\beta_1,t) = \frac{1}{M(N_s+1)}\sum_{1,s}^{M,N_s}\frac{2\sin^2\phi_s}{1+e^{\beta_1(\cos\phi_s+\cos\theta_1)}}\left|I(n,t,N_s+N_b)\right|^2 \qquad (3.35)$$

$$B(\beta_2,t) = \frac{1}{M(N_b+1)}\sum_{1,b}\frac{2\sin^2\phi_b}{1+e^{\beta_2(\cos\theta_1+\cos\phi_b)}}\left|\sum_j\frac{1}{N_s+N_b+1}g(\omega_j,\phi_b,t)\right|^2 \qquad (3.36)$$

In terms of these definitions (3.30) can be written as

$$\langle f_{nm}^\dagger f_{nm}\rangle_t = S(\beta_1,t) + B(\beta_2,t) \qquad (3.37)$$

The limit $|\Omega_B| \to \infty$ will be taken by letting $M,N_b \to \infty$, and this will correspond to the case of Ω_S of finite length N_s, interacting with Ω_B which is of infinite extent. We deal with the two functions S, and B separately.

(i) The limit of the function $S(\beta_1,t)$.

$S(\beta_1,t)$ depends on N_b only through the function $I(n,t,N_s+N_b)$, and on M through the sum over 1. The limit $M \to \infty$ can be dealt with simply by using the definition of the Riemann integral [22] and observing that $I(n,t,N_s+N_b)$ does not depend on θ_1. In this limit the sum over 1 may then be replaced by integration over θ.

$$\underset{M\to\infty}{\text{Lim}}\ S(\beta_1,t)\ =\ \frac{1}{2\pi}\int_0^{2\pi}d\theta\ \frac{1}{N_s+1}\sum_{s=1}^{N_s}\frac{2\sin^2\phi_s}{1+e^{\beta(\cos\theta+\cos\phi_s)}}\ |I(n,t,N_s+N_b)|^2$$

(3.38)

Using the residue theorem and introducing the function

$$K(Z,N_s+N_b)\ =\ (e^{-i2(N_s+N_b+1)Z}-1)^{-1}$$

(3.39)

we can write

$$I(n,t,N_s+N_b)\ =\ \frac{-1}{2\pi}\oint_C\frac{e^{it\cos Z}.\sin\ nZ.\sin(N_s+1)Z}{(\cos Z-\cos\phi_s)(e^{-i2(N_s+N_b+1)Z}-1)}\ dZ$$

(3.40)

Here we have used the fact that the integral in (3.40) has removable

singularities at $Z=\pm\ \phi_s$, 0, π. The contour C is illustrated in figure

3.2
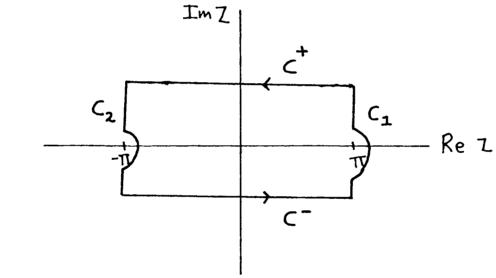
Figure 3.2. The contour C in the Z plane.

The following proposition establishes the limit $N_b\to\infty$ in (3.40).

Proposition 3.1

$$\underset{N_b\to\infty}{\text{Lim}}\ I(n,t,N_s+N_b)\ =\ \frac{1}{2\pi}\int_{C^-}\frac{e^{it\cos Z}.\sin\ nZ.\sin(N_s+1)Z}{\cos Z-\cos\phi_s}\ dZ$$

(3.41)

Proof: The periodic property of the integral in (3.40) implies that

the integrals along C_1, and C_2 are equal and opposite in sign, so contri-

bute zero. The function I is then equal to the integrals along C^+ and C^-.

Now the integrand in (3.40) depends on N_b only through the function $K(Z,N_s+N_b)$, and the limit $N_b \to \infty$ of K on C^+ and C^- is

$$\lim_{N_b \to \infty} K(Z,N_s+N_b) = \begin{cases} 0 & Z \in C^+ \\ -1 & Z \in C^- \end{cases}$$

The function $f(Z,\phi_s,t)$ as defined in (3.32) is continuous on C^+,C^- and is therefore bounded on C^+,C^-. The Limit $N_b \to \infty$ for I is thus easily established to be given by equation (3.41)//.

Combining (3.41) and (3.38) we have the required result

$$\lim_{\substack{M \to \infty \\ N_b \to \infty}} S(\beta_1,t) = \frac{1}{2\pi} \int_0^{2\pi} d\theta \frac{1}{N_s+1} \sum_{s=1}^{N_s} \frac{2\sin^2\phi_s}{1+e^{\beta_1(\cos\theta+\cos\phi_s)}}$$

$$\cdot \left| \frac{1}{2\pi} \int_{C^-} \frac{e^{it\cos Z} \cdot \sin nZ \cdot \sin(N_s+1)Z}{\cos Z-\cos\phi_s} \, dZ \right|^2 \qquad (3.42)$$

(ii) The limit of the function $B(\beta_2,t)$ on $|\Omega_B| \to \infty$.

In order that the limit $N_b \to \infty$ be obtained we rewrite equation (3.36) as

$$B(\beta_2,t) = \frac{1}{2\pi} \int_0^{2\pi} d\theta \left(\frac{1}{N_s+N_b+1}\right)^2 \sum_{j,j'} \frac{1}{N_b+1} \sum_{b=1}^{N_b} g(\omega_j,\phi_b,t) \, g^*(\omega_j',\phi_b,t)$$

$$\cdot \frac{2\sin^2\phi_b}{1+e^{\beta_2(\cos\phi_b+\cos\theta)}} \qquad (3.43)$$

where we have taken the limit $M \to \infty$ by writing the sum over 1 as an integral over θ. Next, using the residue theorem, and introducing the functions $K(Z,N_s+N_b)$, $K(W,N_b)$ as defined in (3.39) we write each sum in (3.43) as a contour integral

$$B(\beta_2,t) = \frac{1}{2\pi}\int\limits_0^{2\pi} d\theta \, \frac{1}{2\pi}\int\limits_C d\lambda \, \frac{1}{2\pi}\int\limits_C dZ \, \frac{1}{2\pi}\int\limits_L dW \, \frac{e^{itcos\lambda}.\sin n\lambda.\sin N_s\lambda}{(cos\lambda-cosW)(e^{-i2(N_s+N_b+1)\lambda}-1)}$$

$$\cdot \, \frac{e^{-itcosZ}.\sin nZ.\sin N_s Z}{(cosZ-cosW)(e^{i2(N_s+N_b+1)W}-1)} \cdot \frac{2\sin^2 W}{1+e^{\beta_2(cosW+cos\theta)}} \cdot \frac{1}{(e^{-i2(N_b+1)W}-1)}$$

$$+ \, \frac{1}{2\pi}\int\limits_0^{2\pi} d\theta \, \frac{1}{2\pi}\int\limits_C d\lambda \, \frac{1}{2\pi}\int\limits_L \frac{dW \, 2e^{-itcosW}.\sin nW.\cos N_s W \, \sin W \, e^{itcos\lambda}.\sin\lambda \, \sin N_s\lambda}{(1+e^{\beta_2(cosW+cos\theta)})(e^{-i2(N_s+N_b+1)\lambda}-1)(cos\lambda-cosW)(e^{-i2(N_b+1)W}-1)}$$

+ complex conjugate

$$+ \, \frac{1}{2\pi}\int\limits_0^{2\pi} d\theta \, (-\frac{1}{2\pi}) \int\limits_L dW \, \frac{2\sin^2 nW.\cos^2 N_s W}{(1+e^{\beta_2(cosW+cos\theta)})(e^{-i2(N_b+1)W}-1)}$$

$$(3.44)$$

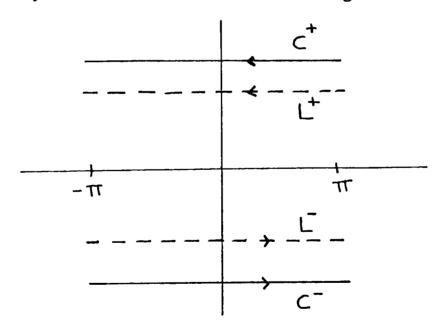The contours C, and L are illustrated in figure 3.3

Figure 3.3. The contours C, and L

As the integrands are periodic the vertical contours vanish by cancellation. C, L, lie in a strip of the complex λ,Z,W planes which is well inside the zeroes of the function $(1+e^{\beta_2(cosW+cos\theta)})$. The following proposition establishes the limit $N_b \to \infty$ in (3.44).

Proposition 3.2

The limit $N_b \to \infty$ of $B(\beta_2, t)$ is given by

$$B(\beta_2, t) = \frac{1}{2\pi} \int_0^{2\pi} d\theta \, \frac{1}{2\pi} \int_{-\pi}^{\pi} d\phi \, \frac{2\sin^2\phi}{1 + e^{\beta_2(\cos\phi + \cos\theta)}}$$

$$\times \left| \frac{e^{it\cos\phi} \cdot \sin n\phi \cdot \cos N_s \phi}{\sin\phi} + \frac{1}{2\pi} \int_{C^-} \frac{e^{it\cos Z} \cdot \sin n Z \cdot \sin N_s Z}{\cos Z - \cos\phi} \, dZ \right|^2$$

(3.45)

Proof: In the integral representation of $B(\beta_2, t)$ as expressed in equation (3.44) the dependence on N_b has been transfered to the functions $K(\lambda, N_s + N_b)$, $K(-Z, N_s + N_b)$, and $K(W, N_b)$. In the limit $N_b \to \infty$ these functions behave as

(i)
$$\lim_{N_b \to \infty} K(\lambda, N_s + N_b) = \begin{cases} -1 & \lambda \in C^- \\ 0 & \lambda \in C^+ \end{cases}$$

(ii)
$$\lim_{N_b \to \infty} K(-Z, N_s + N_b) = \begin{cases} 0 & Z \in C^- \\ -1 & Z \in C^+ \end{cases}$$

(3.46)

(iii)
$$\lim_{N_b \to \infty} K(W, N_b) = \begin{cases} -1 & W \in L^- \\ 0 & W \in L^+ \end{cases}$$

Using (3.46) we obtain the limit $N_b \to \infty$ in (3.44) to be

$$\lim_{N_b \to \infty} B(\beta_2, t) = \frac{1}{2\pi} \int_0^{2\pi} d\theta \, \frac{1}{2\pi} \int_{C^-} d\lambda \, \frac{1}{2\pi} \int_{C^+} dZ \, \frac{1}{2\pi} \int_{L^-} dW \, \frac{e^{it\cos\lambda} \cdot \sin n\lambda \cdot \sin N_s \lambda}{\cos\lambda - \cos W}$$

$$\cdot \frac{e^{-it\cos Z} \cdot \sin n Z \cdot \sin N_s Z}{\cos Z - \cos W} \cdot \frac{2\sin^2 W}{1 + e^{\beta_2(\cos W + \cos\theta)}}$$

$$+ \frac{1}{2\pi} \int_0^{2\pi} d\theta \frac{1}{2\pi} \int_C d\lambda \frac{1}{2\pi} \int_{L^-} dW \frac{e^{-it\cos W}.2\sin W.\sin nW.\cos N_s W.e^{it\cos\lambda}.\sin n\lambda.\sin N_s\lambda}{(1+e^{\beta_2(\cos W+\cos\theta)})(\cos\lambda-\cos W)}$$

+ complex conjugate

$$+ \frac{1}{2\pi} \int_0^{2\pi} d\theta \frac{1}{2\pi} \int_{L^-} dW \frac{2\sin^2 nW.\cos^2 N_s W}{1+e^{\beta_2(\cos W+\cos\theta)}} \qquad (3.47)$$

Cauchy's theorem allows us to move L^- onto the real line, and the continuity of the integrand so defined in its domain allows the order of integration to be reversed. Equation (3.47) is then identical to (3.45) which proves the proposition.//

Thus we have

$$\langle f_{nm}^\dagger f_{nm} \rangle_t = S(\beta_1,t) + B(\beta_2,t) \qquad (3.48)$$

where S, and B are given by (3.42) and (3.45).

3. The time evolution and approach to equilibrium

Equation (3.48) describes the time evolution of the observable $f_{nm}^\dagger f_{nm}$ of the finite Ω_S, when it is in interaction with a heat bath of infinite extent relative to Ω_S. We want to examine two limiting cases

(a) Time $t = 0$. This should correspond to the situation when Ω_S, and the heat bath are initially isolated. $\langle f_{nm}^\dagger f_{nm} \rangle_{t=0}$ should then be the initial equilibrium state of Ω_S.

(b) Time $t \to \infty$. In this case the final state of Ω_S is obtained when the interaction is complete.

Case a.

Substituting for $t = 0$ in $S(\beta_1,t)$ and $B(\beta_2,t)$ and evaluating the integrals (see Appendix A) for $1 \leq n \leq N_s$

$$\frac{1}{2\pi} \int_{-\pi}^{\pi} \frac{\sin(N_s+1)W.dW}{\cos W-\cos\phi_s} = (-)^{s+1} \frac{\sin n\phi_s}{\sin\phi_s} \qquad (3.49)$$

$$\frac{1}{2\pi} \text{ P}\int_{-\pi}^{\pi} \frac{\sin nw . \sin N_s w}{\cos w - \cos \phi} dw = \frac{\sin n\phi . \cos N_s \phi}{\sin \phi}$$

we obtain for S and B

$$S(\beta_1, t=0) = \frac{1}{2\pi} \int_0^{2\pi} d\theta \frac{1}{N_s+1} \sum_{s=1}^{N_s} \frac{2\sin^2 n\phi_s}{1+e^{\beta_1(\cos\phi_s + \cos\theta)}} \qquad (3.50)$$

$$B(\beta_2, t=0) = 0$$

This result, as expected means

$$<f_{nm}^\dagger f_{nm}>_{t=0} = \frac{1}{2\pi} \int_0^{2\pi} d\theta \frac{1}{N_s+1} \sum_{s=1}^{N_s} \frac{2\sin^2 n\phi_s}{1+e^{\beta_1(\cos\phi_s + \cos\theta)}} \qquad (3.51)$$

which is the initial equilibrium state, with all contributions from Ω_B vanishing.

Case b.

We can investigate the limit $t \to \infty$ by analysing the asymptotic behaviour of the time dependent integrals in (3.48). Firstly we see that $S(\beta_i, t)$ depends on time through the integral

$$I(t) = \frac{1}{2\pi} \text{ P}\int_{-\pi}^{\pi} \frac{e^{it\cos w} . \sin nw . \sin(N_s+1)w}{\cos w - \cos\phi_s} dw \qquad (3.52)$$

Using the fact that $w = \phi_s$ as a removable singularity and that

$$\sin(N_s+1)w = 2^{N_s} . \sin w \prod_{s=1}^{N_s} (\cos w - \cos\phi_s) \qquad (3.53)$$

we can write I(t) as

$$I(t) = \frac{1}{\pi} \sum_{l=1}^{N_s} C_{ls} \int_0^\pi e^{it\cos\omega} . \sin n\omega . \sin l\omega \, d\omega \qquad (3.54)$$

The integral representation of Bessel functions of the first kind [23]

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$$J_n(t) = \frac{i^{-n}}{\pi} \int_0^\pi e^{it\cos\omega} \cdot \cos n\,\omega \cdot d\omega \qquad (3.55)$$

implies

$$I(t) = \sum_{l=1}^{N_s} (K_{ls}\, J_{n-1}(t) + K'_{ls}\, J_{n+1}(t)) \qquad (3.56)$$

Asymptotically the $J_n(t)$ decay to zero at like $t^{-\frac{1}{2}}$:

$$I(t) \underset{\sim}{\overset{t\to\infty}{}} ct^{-\frac{1}{2}} \qquad (3.57)$$

Thus $S(\beta_1,t)$ decays to zero at the rate, t^{-1}

$$\underset{t\to\infty}{\text{Lim}}\ S(\beta_1,t) = 0 \qquad (3.58)$$

The time dependence of $B(\beta_2,t)$ is given by

$$P(t) = \frac{e^{it\cos\phi}\cdot\sin n\phi\cdot\cos N_s\phi}{\sin\phi} + \frac{1}{2\pi} \int_{C^-} \frac{e^{it\cos Z}\cdot\sin nZ\cdot\sin N_s Z\ dZ}{\cos Z - \cos\phi}$$

$$(3.59)$$

Using the residue theorem

$$P(t) = \frac{e^{it\cos\phi}\cdot e^{iN_s\phi}}{\sin\phi} \cdot \sin n\phi + \frac{1}{2\pi} \int_{C'} \frac{e^{it\cos Z}\cdot\sin nZ\cdot\sin N_s Z\ dZ}{\cos Z - \cos\phi}$$

$$(3.60)$$

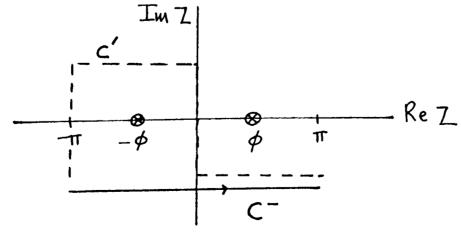where C^-, and C' are illustrated in figure (3.4)

Figure 3.4. The contours C^-, C' in the Z plane

Asymptotically P(t) behaves as

$$P(t) \underset{\sim}{\overset{t \to \infty}{}} \frac{e^{itcos\phi} \, e^{iN_s\phi} \cdot sinn\phi}{sin\phi} + O(t^{-1})$$ (3.61)

Equation (3.61) establishes the limit $t \to \infty$ of $B(\beta_2,t)$

$$\underset{t \to \infty}{Lim} B(\beta_2,t) = \frac{1}{2\pi^2} \int_0^{2\pi} d\theta \int_0^{\pi} d\phi \frac{2sin^2n\phi}{1+e^{\beta_2(cos\theta+cos\phi)}}$$ (3.62)

Combining (3.58) and (3.62) we obtain

$$\underset{t \to \infty}{Lim} <f_{nm}^{\dagger}f_{nm}>_t = \frac{1}{2\pi^2} \int_0^{2\pi} \int_0^{\pi} \frac{2sin^2n\phi \, d\phi.d\theta}{1+e^{\beta_2(cos\theta+cos\phi)}}$$ (3.63)

which is the new equilibrium state of $f_{nm}^{\dagger}f_{nm}$ in Ω_S. It is clear, that as long as Ω_S is finite relative to Ω_B, then Ω_S will approach the new equilibrium state. To comment on the effect of the size of Ω_S, we note that the integrals $I(t)$, and $P(t)$ do not converge uniformly in N_S, the length of Ω_S. This means the larger the Ω_S, the longer we have to wait for equilibrium. Moreover by making Ω_S sufficiently large, so that well away from the edges of the lattice we obtain the translationally invariant state

$$Lim <f_{nm}^{\dagger}f_{nm}>_t = \frac{1}{2\pi^2} \int_0^{2\pi} \int_0^{\pi} \frac{d\phi.d\theta}{1+e^{\beta_2(cos\theta+cos\phi)}}$$ (3.64)

(i) $t \to \infty$

(ii) Ω_S, $n \to \infty$

The main conclusion from this Chapter is that, local thermal deviations from equilibrium confined to a region Ω_S of an infinite lattice Ω, $\Omega_S \subset \Omega$, relax to the equilibrium state of Ω characterised by the temperature of Ω, β_2. This is in accordance with the, C*-algebraic

results of Emch and Radin [18], this model providing a particular example for which their theory is valid.

CHAPTER IV. TIME EVOLUTION (GENERAL CASE)

In Chapter III we analysed the time dependent properties of $<f^\dagger_{nm} f_{nm}>_t$ for the special case where the parameter γ, which scales the interaction strength between Ω_S, and Ω_B was set equal to one. We found that Ω_S interacting with the 'infinite' heat bath Ω_B, approached its new equilibrium state, that is that of the heat bath, at a rate proportional to t^{-1}. In this Chapter we would like to ask; how do these results depend on the parameter γ and do the conclusions arrived at in Chapter III still hold good? In order that we answer these questions we calculate $<f^\dagger_{nm} f_{nm}>_t$ for the case of arbitrary γ. To do this we note that the cylindrical symmetry of the lattice is still present, and that the eigenvalues of the total Hamiltonian of the lattice Ω as given by (3.4) take the general form

$$\Lambda_{j1} = \lambda_j + \cos\theta_1. \tag{4.1}$$

Here λ_j are the new perturbed frequencies corresponding to the motion in the $\hat{n}$ direction of the lattice Ω, with

$$\lambda_j = \cos\omega_j \text{ for } \gamma = 1 \tag{4.2}$$

Furthermore equation (3.30) is still valid, with the exception that now we must redefine the T_{nj}, U_{js}, and U_{jb}, which will in general depend on γ.

The problem of obtaining the equations of motion for $<f^\dagger_{nm} f_{nm}>_t$ for the general case of arbitrary γ is thus reduced to find expressions for λ_j, $T_{nj}(\gamma)$, $U_{js}(\gamma)$, $U_{jb}(\gamma)$.

1. The Eigenvalues λ_j

To simplify the derivation of equations for λ_j, U_{js}, U_{jb}, and T_{nj} we consider the equivalent one dimensional problem

$$H_T = \frac{1}{2} \sum_{n\epsilon\Omega_S} (F^\dagger_{n+1} F_n + h.c) + \frac{1}{2} \sum_{n\epsilon\Omega_B} (F^\dagger_{n+1} F_n + h.c)$$

$$+ \frac{\gamma}{2} (F^\dagger_{N_S} F_{N_S+1} + h.c). \tag{4.3}$$

The eigenvalues of (4.3) will then be the required λ_j. Equation (4.3) is now written in the representation where $H(\Omega_S)$ and $H(\Omega_B)$ are diagonal. Using transformation (3.10) we obtain

$$H_\tau = \sum_{s=1}^{N_s} \cos\phi_s \sigma_s^\dagger \sigma_s + \sum_{b=1}^{N_b} \cos\phi_b \cdot \eta_b^\dagger \eta_b$$

$$+ \gamma \left((N_s+1)(N_b+1)\right)^{-\frac{1}{2}} \sum_{s,b}^{N_s,N_b} \sin N_s\phi_s \cdot \sin\phi_b \; (\sigma_s^\dagger \eta_b + \text{h.c}) \quad (4.4)$$

Equation (4.4) is reduced to diagonal form by requiring that the new fermion operators which diagonalise H_τ, satisfy

$$[H_\tau, X_j^\dagger]_- = \lambda_j X_j^\dagger \quad (4.5)$$

Here, as in (3.18) we seek the new U_{js}, and U_{jb} so that

$$X_j^\dagger = \sum_s U_{js}\sigma_s^\dagger + \sum_b U_{jb}\eta_b^\dagger \quad (4.6)$$

Substituting (4.4) and (4.6) in (4.5) we obtain the coupled equations

$$(\lambda_j - \cos\phi_s)\, U_{js} = \frac{\gamma}{\left[(N_s+1)(N_b+1)\right]^{\frac{1}{2}}} \sum_{b=1}^{N_b} \sin N_s\phi_s \cdot \sin\phi_b \; U_{jb}$$
$$(4.7)$$

$$(\lambda_j - \cos\phi_b)\, U_{jb} = \frac{\gamma}{\left[(N_s+1)(N_b+1)\right]^{\frac{1}{2}}} \sum_{s=1}^{N_s} \sin N_s\phi_s \cdot \sin\phi_b \; U_{js}$$

To solve for U_{js} and U_{jb} we introduce the functions

$$A_j = \sum_{b=1}^{N_b} \left(\frac{2}{N_b+1}\right)^{\frac{1}{2}} \cdot \sin\phi_b \; U_{jb} \quad (4.8)$$

$$B_j = \sum_{s=1}^{N_s} \left(\frac{2}{N_s+1}\right)^{\frac{1}{2}} \cdot \sin N_s\phi_s \; U_{js}$$

in terms of which (4.7) becomes

$$U_{js} = \frac{\gamma}{2} \left(\frac{2}{N_s+1}\right)^{\frac{1}{2}} \frac{\sin N_s \phi_s}{\lambda_j - \cos \phi_s} A_j \qquad (a)$$

$$(4.9)$$

$$U_{jb} = \frac{\gamma}{2} \left(\frac{2}{N_b+1}\right)^{\frac{1}{2}} \frac{\sin \phi_b}{\lambda_j - \cos \phi_b} B_j \qquad (b)$$

Here we have assumed that all the eigenvalues of $H(\Omega_S)$ and $H(\Omega_B)$ are

perturbed by the interaction, ie $\lambda_j \neq \cos\phi_s$, $\neq \cos\phi_b$.

We now multiply (4.9)a by $\left(\frac{2}{N_s+1}\right)^{\frac{1}{2}} \sin N_s \phi_s$, (4.9)b by $\left(\frac{2}{N_b+1}\right)^{\frac{1}{2}} \sin \phi_b$,

and sum over s, and b respectively to obtain

$$B_j = \frac{\gamma}{N_s+1} \sum_{s=1}^{N_s} \frac{\sin^2 \phi_s}{\lambda_j - \cos \phi_s} A_j$$

$$(4.10)$$

$$A_j = \frac{\gamma}{N_b+1} \sum_{b=1}^{N_b} \frac{\sin^2 \phi_b}{\lambda_j - \cos \phi_b} B_j$$

For non trivial solutions of (4.10) we demand

$$\begin{vmatrix} -1 & \gamma \, G_{N_s}(\lambda_j) \\ \gamma \, G_{N_b}(\lambda_j) & -1 \end{vmatrix} = 0 \qquad (4.11)$$

where we used the definitions

$$G_{N_s}(\lambda_j) = \frac{1}{N_s+1} \sum_{s=1}^{N_s} \frac{\sin^2 \phi_s}{\lambda_j - \cos \phi_s}$$

$$(4.12)$$

$$G_{N_b}(\lambda_j) = \frac{1}{N_b+1} \sum_{b=1}^{N_b} \frac{\sin^2 \phi_b}{\lambda_j - \cos \phi_b}$$

From (4.11) the roots of the polynomial $P_{N_s,N_b}(\lambda)$ give the required

spectrum λ_j,

$$P_{N_s,N_b}(\lambda) \;=\; 1 - \gamma^2 \, G_{N_s}(\lambda) \, G_{N_b}(\lambda) \tag{4.13}$$

and as there are $N_s + N_b$ roots, all the eigenvalues λ_j are accounted for by (4.13).

Equations (4.9) for the matrix elements U_{js}, and U_{jb} still contain the unknown A_j, and B_j. We can eliminate these unknowns by applying the required normalisation condition on U_{js}, and U_{jb}, so that the transformation U is unitary. Forming the sum

$$C \;=\; \sum_s |U_{js}|^2 + \sum_b |U_{jb}|^2 \tag{4.14}$$

and using equations (4.13) and (4.10), we have

$$C \;=\; \frac{\gamma^2}{2} \, |A_j|^2 \, G_{N_s}(\lambda_j) \, N^2(\lambda_j)$$

$$\tag{4.15}$$

$$C \;=\; \frac{\gamma^2}{2} \, |B_j|^2 \, G_{N_b}(\lambda_j) \, N^2(\lambda_j)$$

with

$$N^2(\lambda_j) \;=\; \left(\frac{\partial P}{\partial \lambda} \right)_{\lambda=\lambda_j} \tag{4.16}$$

we obtain the normalised matrix elements

$$U_{js} \;=\; \left(\frac{2}{N_s+1}\right)^{\frac{1}{2}} \frac{\sin N_s \phi_s}{\lambda_j - \cos\phi_s} \, [\, 2G_{N_s}(\lambda_j) \, N^2(\lambda_j) \,]^{-\frac{1}{2}} \tag{4.17}$$

$$U_{jb} \;=\; \left(\frac{2}{N_b+1}\right)^{\frac{1}{2}} \frac{\sin\phi_b}{\lambda_j - \cos\phi_b} \, [\, 2G_{N_b}(\lambda_j) \, N^2(\lambda_j) \,]^{-\frac{1}{2}} \tag{4.18}$$

Finally the transformation $T(\gamma)$ which diagonalises (4.3) directly is given by

$$T(\gamma) \;=\; U(\gamma) \begin{pmatrix} S & 0 \\ 0 & B \end{pmatrix} \tag{4.19}$$

where the matrix elements of S and B are defined in (3.12) and (3.13).

As we are interested in $n\epsilon\Omega_S$ we have

$$T_{nj} = (\frac{2}{N_s+1})^{\frac{1}{2}} \sum_{s=1}^{N_s} \sin(N_s-p)\phi_s \cdot U_{sj} \qquad (4.20)$$
$$n\epsilon\Omega_S$$

where we set $n = N_s-p$ with p the distance of the lattice point n from

the interaction boundary at N_s. Explicitly (4.20) is

$$T_{nj} = [2G_{N_s}(\lambda_j) \, N^2(\lambda_j)]^{-\frac{1}{2}} \frac{2}{N_s+1} \sum_{s=1}^{N_s} \frac{\sin(p+1)\phi_s \cdot \sin\phi_s}{\lambda_j-\cos\phi_s}$$
$$n\epsilon\Omega_S$$
$$(4.21)$$

We can now use equations (4.17), (4.18) and (4.21) in (3.30) to obtain the

equations of motion for the case of arbitrary γ.

2.   The Equations of Motion for $<f^\dagger_{nm}f_{nm}>_t$

As before we write

$$<f^\dagger_{nm}f_{nm}>_t = S(\beta_1,t,\gamma) + B(\beta_2, t,\gamma) \qquad (4.22)$$
$$(n,m)\epsilon\Omega_S$$

where we define

$$S(\beta_1,t,\gamma) = \frac{1}{M(N_s+1)} \sum_{1,s} \frac{2\sin^2\phi_s}{1+e^{\beta_1(\cos\phi_s+\cos\theta_1)}}$$

$$\cdot \; |\sum_j \frac{e^{it\lambda_j}}{\lambda_j-\cos\phi_s} \frac{G_{N_s}(p,\lambda_j)}{G_{N_s}(\lambda_j) \, N^2(\lambda_j)}|^2 \qquad (4.23)$$

$$B(\beta_2,t,\gamma) = \frac{1}{M(N_b+1)} \sum_{1,b} \frac{2\sin^2\phi_b}{1+e^{\beta_2(\cos\phi_b+\cos\theta_1)}}$$

$$\cdot \; |\sum_j \frac{\gamma e^{it\lambda_j}}{\lambda_j-\cos\phi_b} \frac{G_{N_s}(p,\lambda_j)}{N^2(\lambda_j)}|^2 \qquad (4.24)$$

and

$$G_{N_s}(p,\lambda_j) = \frac{1}{N_s+1} \sum_{s=1}^{N_s} \frac{\sin(p+1)\phi_s \cdot \sin\phi_s}{\lambda_j - \cos\phi_s} \qquad (4.25)$$

The following proposition proves an important identity, which will be used in the following sections.

Proposition 4.1

The function $G_{N_s}(p,\lambda)$ can be written as the ratio of two Chebyshev polynomials of the second kind [24]

$$G_{N_s}(p,\lambda) = \frac{U_{N_s-p-1}(\lambda)}{U_{N_s}(\lambda)} \qquad (4.26)$$

Proof: We make the substitution $\lambda = \cos\theta$, and with the aid of the Residue theorem write

$$G_{N_s}(p,\cos\theta) = \frac{1}{2\pi} \oint_C \frac{\sin(p+1)Z \cdot \sin Z \cdot dZ}{(\cos\theta-\cos Z)(e^{i2(N_s+1)Z}-1)}$$

$$- \frac{\cos(N_s+1)\theta}{\sin(N_s+1)\theta} \cdot \sin(p+1)\theta \qquad (4.27)$$

The contour C is illustrated in Figure 4.1.
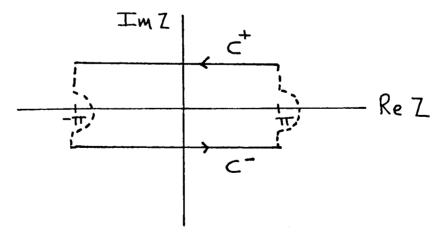

Figure 4.1.

The following observations are readily verified

(i) Singularities at $Z=0$, $\pm\pi$ are removable.

(ii) The second term in (4.27) is the residue at $Z = \pm\theta$.

(iii) The vertical contours (dotted lines) vanish, due to periodicity

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of the integrand.

(iv) The integral along C^- can be made to vanish by taking the limit $\alpha \to \infty$ where $Z = (x - i\alpha) \in C^-$.

(v) The integral I, along C^+ can be explicitly evaluated (see Appendix B)

$$I = \cos(p+1)\theta$$

Using these properties and (4.27) the proposition can be established from the identity [24]

$$U_n(\cos\theta) = \frac{\sin(n+1)\theta}{\sin\theta} \quad //$$

As discussed in Chapter III interest now lies in the limit $|\Omega_B| \to \infty$, and the next section establishes the form of the functions S, and B in this limit.

3. The Limit $|\Omega_B| \to \infty$

The time dependence of the functions S, B is given by a sum over the eigenvalues λ_j, and it is pertinent at this stage to examine the spectral properties of H_τ in the limit $|\Omega_B| \to \infty$. Propositions (4.2) and (4.3) establish these properties.

Proposition 4.2

The limit of $P_{N_s,N_b}(\lambda)$ as $N_b \to \infty$ is given by

$$P_{N_s,\infty}(\lambda) = 1 - \gamma^2 G_{N_s}(\lambda)(\lambda - \sqrt{\lambda^2 - 1}) \qquad (4.28)$$

Proof:

(i) Using the definition of a Riemann integral, the summation over b in (4.13) is replaced by integration over ϕ

$$P_{N_s,\infty}(\lambda) = 1 - \gamma^2 G_{N_s}(\lambda) \cdot \frac{1}{2\pi} \int_{-\pi}^{\pi} \frac{\sin^2\phi}{\lambda - \cos\phi} \cdot d\phi \qquad (4.29)$$

(ii) The integral (4.28) converges uniformly to

$$\frac{1}{2\pi} \int_{-\pi}^{\pi} \frac{\sin^2\phi}{\lambda - \cos\phi} \cdot d\phi = (\lambda - \sqrt{\lambda^2 - 1}) \qquad (4.30)$$

in the cut $[-1,1]\lambda$ plane with choice of branch given by $(\lambda^2-1)^{\frac{1}{2}} > 0$

$\lambda > 0$ //

Equation (4.28) gives the spectral properties of H_τ in the limit $|\Omega_B| \to \infty$.

Proposition 4.3

The spectral properties of H_τ as a function of the parameter γ can be classified into two cases.

(i) $P_{N_s, \infty}(\lambda)$ has no real zeroes in which case H_τ has a continuous spectrum, represented by the cut in the complex λ plane from $[-1,1]$. This corresponds to the range of values $\gamma^2 \leq 1$.

(ii) $P_{N_s, \infty}(\lambda)$ has real zeroes, which means that the spectrum of H_τ consists of continuous and discrete parts. The range of values $\gamma^2 > 1$ results in this case. It is important at this stage to realise that these real roots can lie on either sheet of the Riemann surface, and that

(a) $\frac{N_s + 1}{N_s} > \gamma^2 > 1$ real roots lie on the sheet with branch $(\lambda^2-1)^{\frac{1}{2}} < 0$ for $\lambda > 0$.

(b) $\gamma^2 > \frac{N_s + 1}{N_s}$ real roots lie on the sheet with branch $(\lambda^2-1)^{\frac{1}{2}} > 0$ for $\lambda > 0$, when $\gamma^2 = 1 + 1/N_s$ the roots lie on the branch points $\lambda = \pm 1$.

Proof: Using (4.26) for the case $p = 0$ we obtain

$$P_{N_s, \infty}(\lambda) = \frac{U_{N_s}(\lambda) - \gamma^2 U_{N_s - 1}(\lambda)(\lambda - \sqrt{\lambda^2 - 1})}{U_{N_s}(\lambda)} \qquad (4.31)$$

Here without ambiguity we write N for N_s. Making the transformation $\lambda = \frac{1}{2}(Z + Z^{-1})$ (4.31) becomes

$$P_{N,\infty}\left(\tfrac{1}{2}(Z+Z^{-1})\right) = \frac{\dfrac{Z^{2(N+1)} - \gamma^2 Z^{2N} + \gamma^2 - 1}{N}}{(Z^2-1)\displaystyle\sum_{h=0} Z^{2n}} \qquad (4.32)$$

The real roots of the function $Q(Z)$

$$Q(Z) = Z^{2(N+1)} - \gamma^2 Z^{2N} + \gamma^2 - 1 \qquad (4.33)$$

correspond to the discrete part of the spectrum of H_τ. Figure 4.2 shows $Q(Z)$ as a function of Z for various regions of γ values
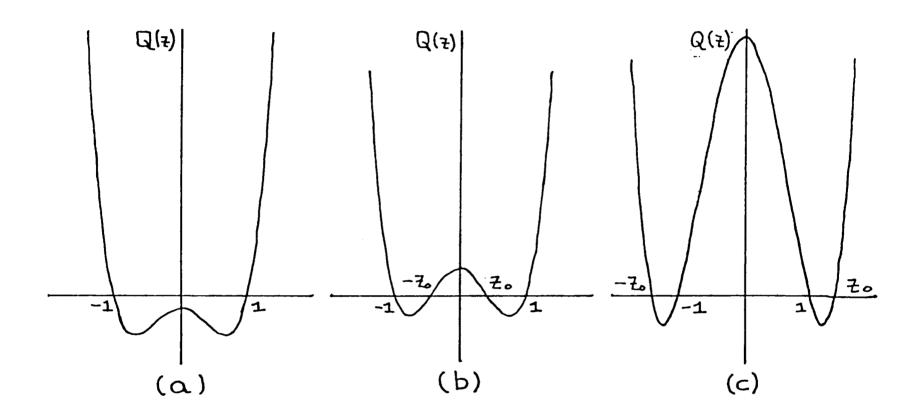

Figure 4.2. Case (a) $\gamma^2 < 1$. (b) $1 < \gamma^2 < 1 + \dfrac{1}{N}$. (c) $\gamma^2 > 1 + \dfrac{1}{N}$

As the roots $Z = \pm 1$ are removable it is easy to establish the following

(i) $\gamma^2 < 1$, $P_{N,\infty}(\lambda)$ has no real roots.

(ii) $1 < \gamma^2 < 1 + \dfrac{1}{N}$ $P_{N,\infty}(\lambda)$ has two real roots at $\pm\lambda_0$, $|\lambda_0| > 1$ on the Riemann surface with branch $(\lambda^2-1)^{\frac{1}{2}} < 0$ $\lambda > 0$.

(iii) $\gamma^2 \geq 1 + \dfrac{1}{N}$ $P_{N,\infty}(\lambda)$ has two real roots at $\pm\lambda_0$, $|\lambda_0| \geq 1$ on the Riemann surface with branch $(\lambda^2-1)^{\frac{1}{2}} > 0$, $\lambda > 0$.

Note that case $\gamma^2 = 1+\frac{1}{N}$ corresponds to the case $\lambda_0 = \pm 1$, that is the simple roots lie on the branch points. This concludes the proof of the properties of $P_{N,\infty}(\lambda)$ as a function of γ. //

In proposition 4.2 the choice of branch $(\lambda^2-1)^{\frac{1}{2}}>0, \lambda>0$ was made. This choice, together with proposition (4.3) establish that $P_{N,\infty}(\lambda)$ does not have any real roots on the Riemann surface so chosen for $\gamma^2<1+\frac{1}{N}$.

We are now in a position to obtain the limiting forms of $S(\beta_1,t,\gamma)$ and $B(\beta_2,t,\gamma)$ when $M, N_b \to \infty$. We shall first consider $S(\beta,t,\gamma)$. This function depends on N_b through the sum

$$I(N_b) = \sum_j \frac{e^{it\lambda_j}}{\lambda_j-\cos\phi_s} \frac{G_{N_s}(p,\lambda_j)}{G_{N_s}(\lambda_j) N^2(\lambda_j)} \qquad (4.34)$$

As a matter of notation the dependence of I on the other parameters t, γ, N_s, etc will be suppressed unless the discussion concerns them directly. With the aid of equation (4.16) and the residue theorem $I(N_b)$ takes the integral representation

$$I(N_b) = \frac{1}{2\pi i} \oint_C \frac{e^{it\lambda}}{(\lambda-\cos\phi_s)} \frac{G_{N_s}(p,\lambda)d\lambda}{G_{N_s}(\lambda)P_{N_s,N_b}(\lambda)} - \text{Res. } \{\text{at } G_{N_s}(\lambda) = 0\} \cdot$$

$$(4.35)$$

The contour C is an ellipse which encloses all the poles of the Integrand in (4.35). The dependence on N_b occurs now only through the function $P_{N_s,N_b}(\lambda)$. Proposition (4.2) now establishes the limit $N_b \to \infty$

$$I(\infty) = \frac{1}{2\pi i} \oint_C \frac{e^{it\lambda}}{\lambda-\cos\phi_s} \frac{G_{N_s}(p,\lambda)d\lambda}{G_{N_s}(\lambda),P_{N_s,\infty}(\lambda)} - \text{Res } \{\text{at } G_{N_s}(\lambda) = 0\}$$

$$(4.36)$$

It is important to realise that the contour C now lies on the Riemann surface chosen by the branch $(\lambda^2-1)^{\frac{1}{2}}>0, \lambda > 0$.

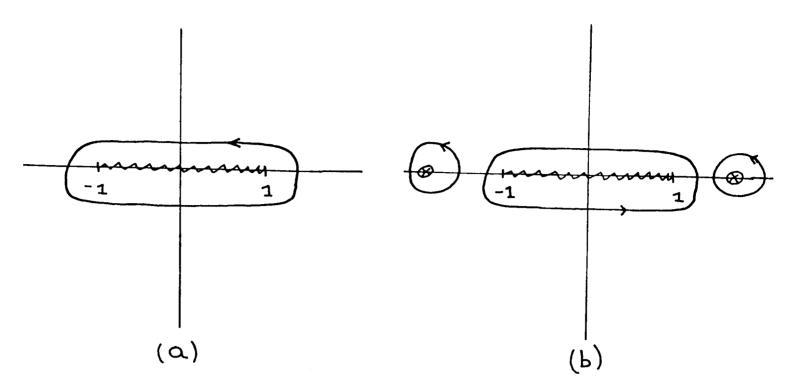Figure (4.3) shows the contour C for two regions of γ values.

(a)   (b)

Figure 4.3.   Contour C on Riemann surface $(\lambda^2-1)^{\frac{1}{2}}>0$, $\lambda > 0$.

$$\text{(a)} \quad \gamma^2<1 + \frac{1}{N_s} , \qquad \text{(b)} \quad \gamma^2>1 + \frac{1}{N_s}$$

As was clear from the discussion of proposition (4.3), in the region $\gamma^2>1 + \frac{1}{N_s}$ two real zeroes of $P_{N,\infty}(\lambda)$ appear on the Riemann sheet where the contour C lies, and that these correspond to discrete eigenvalues of the Hamiltonian H_τ. This is the situation illustrated in figure 4.3(b). The region $1<\gamma^2< 1 + \frac{1}{N_s}$, corresponds to the real zeroes of $P_{N_s,\infty}(\lambda)$, which lie on the Riemann sheet with $(\lambda^2-1)^{\frac{1}{2}}<0$, $\lambda \geqslant 0$, and that these may be ignored. It is worth noting that this region depends on the size N_s of the system as $1 + \frac{1}{N_s}$, ie the larger the system Ω_s, the smaller the region $[1,1 + \frac{1}{N_s})$. The consequences on the time evolution of the isolated eigenvalues will be discussed in the next section.

Using (4.23) we can now write the limit of $M,N_b\to\infty$ of $S(\beta_1,t,\gamma)$ as

$$S(\beta,t,\gamma) = \frac{1}{2\pi} \int_0^{2\pi} d\theta \frac{i}{N_s+1} \sum_{s=1}^{N_s} \frac{2\sin^2\phi_s}{1+e^{\beta_1(\cos\phi_s+\cos\theta)}} |I(\infty)|^2$$

(4.37)

where $I(\infty)$ is given by (4.36).

To deal with the function $B(\beta_2,t,\gamma)$ in the limit $M,N_b \to \infty$ we rewrite equation (4.24) as

$$B(\beta_2,t,\gamma) = \frac{1}{2\pi} \int_0^{2\pi} d\theta \sum_j \sum_{j'} \frac{1}{N_b+1} \sum_{b=1}^{N_b} \frac{\gamma e^{it\lambda_j}}{\lambda_j - \cos\phi_b} \cdot \frac{\gamma e^{-it\lambda_{j'}}}{\lambda_{j'} - \cos\phi_b}$$
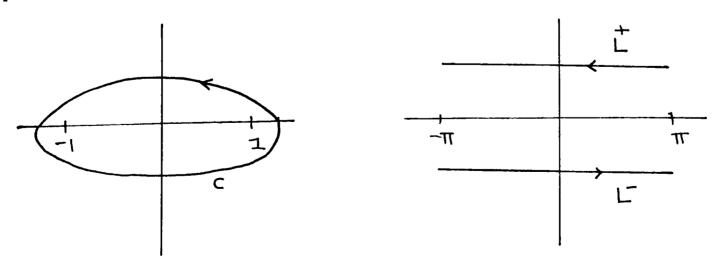
$$\cdot \frac{G_{N_s}(p,\lambda_j)}{N^2(\lambda_j)} \cdot \frac{G_{N_s}(p,\lambda_{j'})}{N^2(\lambda_{j'})} \cdot \frac{2\sin^2\phi_b}{1+e^{\beta_2(\cos\phi_b+\cos\theta)}} \qquad (4.38)$$

where we have taken the limit $M \to \infty$ by replacing $\frac{1}{M}\sum_1$ by the integration over θ. Using the property (4.16) and introducing the function $K(Z,N_b) = (e^{-i2(N_b+1)Z}-1)^{-1}$, we write with the aid of the residue theorem

$$B(\beta_2,t,\gamma) = \frac{1}{2\pi} \int_0^{2\pi} d\theta \frac{1}{2\pi i} \oint_C d\lambda \frac{1}{2\pi i} \oint_C d\lambda' \left(-\frac{1}{2\pi}\right) \int_L dZ \frac{\gamma e^{it\lambda} G_{N_s}(p,\lambda)}{(\lambda-\cos Z)P_{N_s,N_b}(\lambda)}$$

$$\cdot \frac{\gamma e^{-it\lambda'} G_{N_s}(p,\lambda')}{(\lambda'-\cos Z)P_{N_s,N_b}(\lambda')} \cdot \frac{2\sin^2 Z}{1+e^{\beta_2(\cos Z+\cos\theta)}} \cdot K(Z,N_b)$$

$$(4.39)$$

The contours C are ellipses enclosing the roots of $P_{N_s,N_b}(\lambda)$ in the λ,λ' planes. The contour L is illustrated in figure (4.4)

(a) Contour C in λ,λ' planes   (b) Contour L in Z plane

Figure 4.4

The contours L, are arranged so that $\lambda = \cos Z$ is an ellipse inside C in the λ, λ' planes for $Z \in L$, that is the poles $\lambda = \cos Z$ lie <u>inside</u> C. In addition L^+, and L^- lie well inside any of the zeroes of $(1+e^{\beta_2(\cos Z+\cos\theta)})$. The vertical parts of the contours in figure 4.4b have been omitted, this being due to straightforward cancellation which results from the periodicity of the integrand in (4.39). In this representation of $B(\beta_2, t, \gamma)$ the N_b dependence has been transferred to the functions $P_{N_s, N_b}(\lambda)$, and $K(Z, N_b)$. The limit $N_b \to \infty$ can now be obtained by using proposition (4.2) and noting that

$$\lim_{N_b \to \infty} K(Z, N_b) = \begin{array}{l} -1, \quad Z \in L^- \\[2mm] 0 \quad Z \in L^+ \end{array} \qquad (4.40)$$

$$\lim_{N_b \to \infty} B(\beta_2, t, \gamma) = \frac{1}{2\pi} \int_0^{2\pi} d\theta \, \frac{1}{2\pi} \int_{-\pi}^{\pi} d\phi \, \frac{2\sin^2\phi}{1+e^{\beta_2(\cos\phi+\cos\theta)}}$$

$$\cdot \frac{\gamma}{2\pi i} \oint_C \frac{e^{it\lambda}}{\lambda-\cos\phi} \cdot \frac{G_{N_s}(p,\lambda)d\lambda}{P_{N_s,\infty}(\lambda)} \cdot \frac{\gamma}{2\pi i} \oint_C \frac{e^{-it\lambda}}{\lambda-\cos\phi} \cdot \frac{G_{N_s}(p,\lambda)d\lambda}{P_{N_s,\infty}(\lambda)}$$

$$(4.41)$$

where we used Cauchy's theorem, to move L^- onto the real line, and noting the continuity of the integrands in the domain of integration interchanged the order of integration. Equation (4.41) describes the time evolution of $B(\beta_2, t, \gamma)$ in the limit $(M, N_b \to \infty)$.

4.   <u>The Time Evolution of $\langle f_{nm}^\dagger f_{nm} \rangle_t$</u>

The equation

$$\langle f_{mn}^\dagger f_{mn} \rangle_t = S(\beta_1, \gamma, t) + B(\beta_2, \gamma, t) \qquad (4.42)$$

where S, and B are given by (4.36) and (4.41), describe the time

evolution of an _initially isolated_ finite region, Ω_S of an infinite lattice Ω, $\Omega_S \subset \Omega$, which is at a different temperature, β_1, to the rest of the lattice, β_2. The question we would like to answer is: under what conditions does Ω serve as a physical heat bath for Ω_S, so that in the limit $t \to \infty$ a new equilibrium state is obtained, which is characterised solely by the temperature β_2. To answer this question we examine the behaviour of the two functions S, and B. Before we examine the time dependence it is worth pointing out two special cases, $\gamma = 0$, $\gamma = 1$. The case $\gamma = 0$ corresponds to Ω_S being completely isolated, and it is easy to show that

$$S(\beta_1, t, \gamma=0) = \frac{1}{2\pi} \int_0^{2\pi} d\theta \frac{1}{N_s+1} \sum_s \frac{2\sin^2(N_s-p)\phi_s}{1+e^{\beta_1(\cos\phi_s+\cos\theta)}} \qquad (4.43)$$

$$B(\beta_2, t, \gamma=0) = 0$$

$\gamma = 1$ is the case considered in Chapter III, and again we can show that S, and B reduce to the corresponding functions of Chapter III.

(i) The time dependence of $S(\beta, t, \gamma)$

In the region $\gamma > 1 + \frac{1}{N_s}$ the contour C in eqn. (4.36) encloses the two real isolated poles on the Riemann sheet $(\lambda^2-1)^{\frac{1}{2}} > 0$, $\lambda > 0$ and as a consequence this implies that $S(\beta, t, \gamma)$ will have a _non vanishing_ limit of $t \to \infty$. This means that no approach to equilibrium is possible in the region $\gamma^2 > 1 + \frac{1}{N_s}$. We now focus our attention to the region $\gamma^2 < 1 + \frac{1}{N_s}$. The mapping $\lambda = \cos\psi$ maps the top sheet of the Riemann surface $(\lambda^2-1)^{\frac{1}{2}} > 0$, $\lambda > 0$ onto a region of the complex ψ plane defined by Re $\psi \in [-\pi, +\pi]$ and Im $\psi \in [0, -\infty]$. The integral (4.36) can thus be transformed to

$$I(t) = \frac{-1}{2\pi i} \int_{\Gamma^-} \frac{e^{it\cos\psi}.\sin(N_s-p)\psi.\sin(N_s+1)\psi.\sin\psi.d\psi}{(\cos\psi-\cos\phi_s).\sin N_s\psi(\sin(N_s+1)\psi-\gamma^2\sin N_s\psi e^{-i\psi})}$$

$$- \text{Res } (G_{N_s} (\lambda) = 0) \tag{4.44}$$
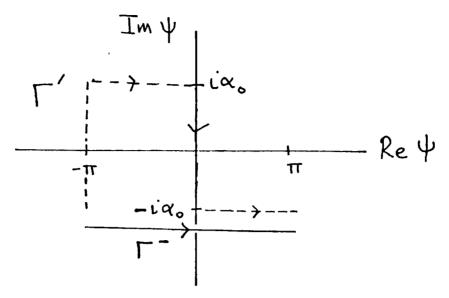
where Γ^- is illustrated in figure 4.4

Figure 4.4. Γ', Γ^- on the complex ψ plane.

In the region $\gamma^2 < 1 + \frac{1}{N_s}$ the region between Γ^- and the real line is

analytic, the integrand having simple poles at $\psi = \pm \pi$, 0, $\pm \phi_s$ being

removable singularities. Using the residue theorem

$$I(t) = \frac{-1}{2\pi i} \int_{\Gamma'} \frac{e^{it\cos\psi} . \sin(N_s-p)\psi . \sin(N_s+1)\psi . \sin\psi \ d\psi}{(\cos\psi-\cos\phi_s) . \sin N_s\psi(\sin(N_s+1)\psi - \gamma^2 \sin N_s\psi e^{-i\psi})}$$

$$\tag{4.45}$$

The value of $\alpha_o > 0$ depends on the value of $\gamma^2 \ \epsilon[1,1 + \frac{1}{N_s})$. The integral

$I(t)$ tends to zero on Γ' as $t \to \infty$

$$I(t) \underset{\sim}{\overset{t \to \infty}{}} t^{-1} \tag{4.46}$$

We can therefore conclude that

$$\underset{t \to \infty}{\text{Lim}} S(\beta_1, t, \gamma^2 < 1 + \frac{1}{N_s}) = 0 \tag{4.47}$$

It is more difficult to decide the type of behaviour at the boundary

$\gamma^2 = 1 + \frac{1}{N_s}$, and this case will not be considered here.

(ii) The time dependence of $B(\beta_2, t, \gamma)$

Again we focus our attention to the region $\gamma^2 < 1 + \frac{1}{N_s}$. Using the

mapping $\lambda = \cos\psi$ the time dependent integrals in (4.41) can be written as

$$P(t) = \frac{-\gamma}{2\pi i} \int_{\Gamma^-} \frac{e^{it\cos\psi}.\sin(N_s-p)\psi.\sin\psi.d\psi}{(\cos\psi-\cos\phi)(\sin(N_s+1)\psi-\gamma^2\sin N_s\psi e^{-i\psi})}$$

(4.48)

where the contours Γ^- and Γ' are illustrated in Figure 4.5
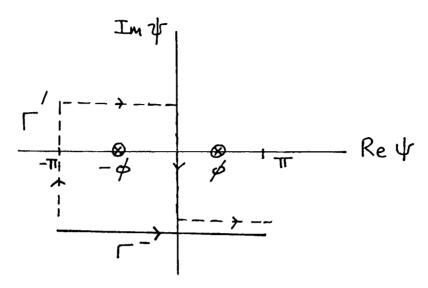

Figure 4.5. Contours Γ^-, Γ' in the complex ψ plane

Using the residue theorem

$$P(t) = \frac{\gamma e^{it\cos\phi}.\sin(N_s-p)\phi}{\sin(N_s+1)\phi-\gamma^2\sin N_s\phi e^{i\phi}} - \frac{\gamma}{2\pi i}\int_{\Gamma'}\frac{e^{it\cos\psi}.\sin(N_s-p)\psi.\sin\psi.d\psi}{(\cos\psi-\cos\phi)(\sin(N_s+1)\psi-\gamma^2\sin N_s\psi e^{-i\psi})}$$

(4.49)

where again for large times

$$P(t) \underset{\sim}{\overset{t\to\infty}{}} \frac{\gamma e^{it\cos\phi}.\sin(N_s-p)\phi}{\sin(N_s+1)\phi-\gamma^2\sin N_s\phi e^{i\phi}} + ct^{-1}$$

(4.50)

Using (4.50) the limit $t \to \infty$ of $B(\beta_2,t,\gamma^2 < 1 + \frac{1}{N_s})$ is obtained

$$\underset{t\to\infty}{\text{Lim}} B(\beta_2,t,\gamma) = \frac{1}{2\pi^2}\int_0^{2\pi} d\theta \int_{-\pi}^{\pi} d\phi \frac{2\sin^2\phi}{1+e^{\beta_2(\cos\phi+\cos\theta)}} \left| \frac{\gamma\sin(N_s-p)\phi}{\sin(N_s+1)\phi-\gamma^2\sin N_s\phi e^{i\phi}} \right|^2$$

(4.51)

Equation (4.51) gives the new equilibrium state of

$$\langle f^\dagger_{nm} f_{nm} \rangle = \underset{t\to\infty}{\text{Lim}} \ (S(\beta_1,t,\gamma) + B(\beta_2,t,\gamma))$$
$$(n,m)\,\epsilon\,\Omega_S$$

in the region $\gamma^2 < 1 + \dfrac{1}{N_S}$. We can now allow Ω_S to become infinitely

large, to obtain a new translationally invariant state.

The limits $N_S, p \to \infty$ in (4.51) give the new translationally

invariant state, so that

$$\underset{\substack{t\to\infty \\ N_S\to\infty \\ p\to\infty}}{\text{Lim}} \ B(\beta_2,t,\gamma) = \frac{\gamma^2}{2\pi} \int_0^{2\pi} \int_0^{\pi} \frac{\sin^2\phi . d\phi . d\theta}{(1+e^{\beta_2(\cos\phi+\cos\theta)})(1-\cos^2\phi(2\gamma^2-\gamma^4))}$$

$$(4.52)$$

The range of values of γ is now restricted to $\gamma^2 \leq 1$.

The new equilibrium state of $\langle f^\dagger_{nm} f_{nm} \rangle$ is thus given by (4.52), so

that

$$\begin{array}{l}(i) \ \underset{t\to\infty}{\text{Lim}} \\ (ii) \ \Omega_S, p\to\infty\end{array} \langle f^\dagger_{nm} f_{nm} \rangle_t = \frac{\gamma^2}{2\pi^2} \int_0^{2\pi} \int_0^{\pi} \frac{\sin^2\phi . d\phi . d\phi}{(1+e^{\beta_2(\cos\theta+\cos\phi)})(1-\cos^2\phi(2\gamma^2-\gamma^4)}$$

$$(4.53)$$

In order that we check the validity of (1.24) it is necessary to

calculate the equilibrium state obtained by direct evaluation of

$$\begin{array}{l}\langle f^\dagger_{nm} f_{nm} \rangle_{\beta_2} \\ (n,m)\,\epsilon\,\Omega_S \\ (i) \ M, N_b\to\infty \\ (ii) \ N_S\to\infty\end{array} = \frac{1}{M} \sum_1 \sum_j T^2_{nj} \frac{1}{1+e^{\beta_2(\lambda_j+\cos\theta_1)}} \qquad (4.54)$$

with the T_{nj} given by (4.21).

<u>Proposition 4.4</u>

The equilibrium state of $\langle f^\dagger_{nm} f_{nm} \rangle_{\beta_2}$ is given by the right hand

side of (4.53).

<u>Proof:</u> This result is proved using techniques developed earlier

in this Chapter. This is done in Appendix C. The calculation so far
has shown that a 'point' in the finite system attains the equilibrium
state of the heat bath with which it is in interaction. It is of interest
to know what happens to a region $\Omega_\Lambda \subset \Omega_S$, and to this end we examine the
behaviour of

$$< \prod_{\substack{(n,m) \\ \varepsilon\Omega_\Lambda}} f^\dagger_{nm} f_{nm} >_t \qquad (4.55)$$

Proposition 4.5 establishes that (4.55) also obtains the equilibrium
state of the heat bath.

Proposition 4.5

$$\lim_{\substack{M,N_b \to \infty \\ t \to \infty \\ N_s \to \infty}} < \prod_{\substack{(n,m) \\ \varepsilon\Omega_\Lambda}} f^\dagger_{nm} f_{nm} >_t = < \prod_{\substack{(n,m) \\ \varepsilon\Omega_\Lambda}} f^\dagger_{nm} f_{nm} >_{\beta_2} \qquad (4.56)$$

Proof: It is clear that by an almost trivial extension of the
calculation for $<f^\dagger_{nm} f_{nm}>_t$ that

$$\lim_{\substack{|\Omega_B| \to \infty \\ t \to \infty \\ |\Omega_S| \to \infty}} <f^\dagger_{nm} f_{1s}>_t = <f^\dagger_{nm} f_{1s}>_{\beta_2} \qquad (4.57)$$

Next we have,

$$< \prod_{\substack{n,m \\ \varepsilon\Omega_\Lambda}} f^\dagger_{nm} f_{nm} >_t = \text{Tr}(\rho(0) \prod_{\substack{(n,m) \\ \varepsilon\Omega_\Lambda}} f^\dagger_{nm}(t) f_{nm}(t)) \qquad (4.58)$$

where the time dependent operators

$$f_{nm}(t) = e^{iH(\Omega)t} f_{nm} e^{-iH(\Omega)t} \qquad (4.59)$$

and satisfy anticommutation rules.

Using the Wick-Bloch-de-Dominicis theorem (Appendix D) we can
express (4.58) in terms of time dependent pair contractions $<f^\dagger_{nm}(t) f_{1s}(t)>$
with (n,m), $(1,s)$ $\varepsilon\Omega_\Lambda$. From (4.57) and theorem D.1 (4.56) readily follows.

CHAPTER V. CALORIMETRIC BEHAVIOUR

In Chapters III, IV the validity of equation (1.24) was analysed for the model introduced in Chapter II. It was found that a finite system coupled to a heat bath of infinite extent attained the equilibrium state of the heat bath provided the Hamiltonian generating the time evolution did not have discrete eigenvalues as part of its spectrum. This result showed that a <u>local</u> deviation from the equilibrium state of the infinite lattice, to be considered as a heat bath relaxed to equilibrium [25].

In this Chapter we shall examine in more detail some questions which arise from the results of the previous two Chapters. In Section 2 we analyse the behaviour of the relaxation time in the weak coupling limit, and particularly its dependence on the size Ω_S of the observed system. In Section 3 the behaviour of the model as $|\Omega_S| \to \infty$ is examined. This situation will represent the behaviour of the system subject to <u>global</u> differences from the equilibrium state, and we discuss the relevance of the concept of mixing to the ideas of return to, or approach to equilibrium. We start by examining the mixing properties of the Hamiltonian H_τ.

1. Mixing Properties of the Hamiltonian $H_\tau(\Omega)$

By examining the correlation functions for the number operators $A_{nm} \equiv (f_{nm}^\dagger f_{nm})$, we can show that the Hamiltonian H_τ in (3.4) has mixing properties in the sense that

$$\underset{t \to \infty}{\text{Lim}} \langle A_{nm} A_{n'm'}(t) \rangle_\rho = \langle A_{nm} \rangle \langle A_{n'm'} \rangle \qquad (5.1)$$

where A_{nm}, $A_{n'm'}$ act at (n,m), (n',m') on the infinite lattice Ω.

Equation (5.1) shows that two local measurements on the lattice Ω become statistically independent under the action of the motion generated by the Hamiltonian $H_\tau(\Omega)$. Physically this corresponds to the mixing property, described in Chapter I, and corresponds to the fact that

after a sufficiently long time, as a result of the motion the particles on the lattice become "mixed up" from any initial configuration. Equation (5.1) is easily seen to be the same form as (1.25).

The correlation function is given by the expression

$$<A_{nm}(0)A_{n'm'}(t)>_\rho = \text{Tr}(\rho A_{nm} e^{iH_\tau(\Omega)t} A_{n'm'} e^{-iH_\tau(\Omega)t})$$

(5.2)

where ρ is taken to be the equilibrium density operator at some inverse temperature β

$$\rho = e^{-\beta H_\tau(\Omega)} / \text{Tr } e^{-\beta H_\tau(\Omega)}$$

(5.3)

To evaluate (5.2) we use the diagonal form H_τ, and express all other operators in this representation.

$$H_\tau = \sum_{(1,j)} (\cos\theta_1 + \lambda_j) X_{1j}^\dagger X_{1j}$$

(5.4)

where the λ_j are given by the roots of $P_{N_s,N_b}(\lambda)$ as defined by (4.13) and

$$X_{1j}^\dagger = \frac{1}{M^{\frac{1}{2}}} \sum_{m,n} e^{im\theta_1} T_{nj} f_{mn}^\dagger$$

(5.5)

and T_{nj} defined by (4.21) for $n\epsilon\Omega_S$ and by

$$T_{nj} = [2G_{N_b}(\lambda_j) N^2(\lambda_j)]^{-\frac{1}{2}} \frac{2}{N_b+1} \sum_{b=1}^{N_b} \frac{\sin n\phi_b \cdot \sin\phi_b}{\lambda_j - \cos\phi_b}$$

(5.6)

for $n\epsilon\Omega_B$.

With the identity

$$e^{it\Lambda_{1j}X_{1j}^\dagger X_{1j}} X_{1j}^\dagger e^{-it\Lambda_{1j}X_{1j}^\dagger X_{1j}} = e^{it\Lambda_{1j}} X_{1j}^\dagger$$

(5.7)

we can express (5.2) as

$$\langle A_{nm}A_{n'm'}(t)\rangle = \frac{1}{M^2} \sum_{\substack{1,1' \\ k,k'}} \sum_{\substack{j,p \\ q,r}} e^{im(\theta_1-\theta_1')} e^{im'(\theta_k-\theta_{k'})}$$

$$T_{nj}T_{np}T_{n'q}T_{n'r}\, e^{it(\Lambda_{kq}-\Lambda_{k'r})}\, \mathrm{Tr}(\rho\; X_{1j}^{\dagger}X_{1'p}X_{kq}^{\dagger}X_{k'r}) \qquad (5.8)$$

By using the Wick-Bloch-de-Dominicis theorem (Appendix D) the trace in (5.8) can be readily evaluated. Applying the theorem (eqns. D.4, D.5 and D.6), and retaining only non-vanishing terms gives

$$\mathrm{Tr}(\rho\; X_{1j}^{\dagger}X_{1'p}X_{kq}^{\dagger}X_{k'r}) = \langle X_{1j}^{\dagger}X_{1'p}\rangle\langle X_{kq}^{\dagger}X_{k'r}\rangle\, \delta_{11'}\delta_{jp}\delta_{kk'}\delta_{qr}$$

$$+ \langle X_{1j}^{\dagger}X_{k'r}\rangle\langle X_{1'p}X_{kq}^{\dagger}\rangle\, \delta_{1k'}\delta_{jr}\delta_{1'k}\delta_{pq} \qquad (5.9)$$

Substituting and simplifying

$$\langle A_{nm}A_{n'm'}(t)\rangle = \langle A_{nm}\rangle\langle A_{n'm'}\rangle + F_1(t)\,F_2(t) \qquad (5.10)$$

with

$$\langle A_{nm}\rangle = \frac{1}{M}\sum_{1,j}|T_{nj}|^2 \langle X_{1j}^{\dagger}X_{1j}\rangle \qquad \text{(a)}$$

$$\qquad (5.11)$$

$$\langle A_{n'm'}\rangle = \frac{1}{M}\sum_{k,r}|T_{n'r}|^2 \langle X_{kr}^{\dagger}X_{kr}\rangle \qquad \text{(b)}$$

$$F_1(t) = \frac{1}{M}\sum_{1,j} e^{i(m-m')\theta_1}\, T_{nj}T_{n'j}\, e^{-it(\cos\theta_1+\lambda_j)} \langle X_{1j}^{\dagger}X_{1j}\rangle$$

$$\qquad (5.12)$$

$$\langle X_{1j}^{\dagger}X_{1j}\rangle = [\,1+e^{\beta(\cos\theta_1+\lambda_j)}\,]^{-1} \qquad (5.13)$$

$$F_1(t,\beta) = F_2(-t,-\beta) \qquad (5.14)$$

It is clear that (5.11) (a) and (b) represent the uncorrelated equilibrium states of the operators A_{nm} and $A_{n'm'}$ located at (n,m) and (n',m') $\varepsilon\Omega$ respectively. Proposition (4.4) establishes their infinite volume equilibrium states. The time dependent functions $F_1(t)$, and $F_2(t)$ represent the correlation between these two lattice sites, and a study of the asymptotic behaviour of $F_{1,2}(t)$ as $|\Omega| \to \infty$, $t \to \infty$ will show whether $A_{nm}A_{n'm'}$ form a mixing pair of operators.

We concentrate on $F_1(t)$, the analysis for $F_2(t)$ is seen from (5.14) to be identical. The transformation coefficients T_{nj} in (5.12) are to be chosen from (4.21) or (5.6) according to whether n,n' belong to Ω_S, or Ω_B. For definitness we choose n,n' $\varepsilon\Omega_S$ so that the T_{nj} are given by (4.21). Then replacing the sum over l by an integral over θ for the limit M $\to \infty$, and using the techniques described in Chapter IV, $F_1(t)$ can be given the integral representation

$$F_1(t) = \frac{1}{2\pi} \int_0^{2\pi} d\theta\, e^{i(m-m')\theta} e^{-it\cos\theta} \frac{1}{2\pi i} \left[\oint_C \frac{d\lambda\, e^{-it\lambda} G_{N_s}(p,\lambda) G_{N_s}(p',\lambda)}{\beta(\cos\theta+\lambda) [1+e^{}] G_{N_s}(\lambda) P_{N_s,N_b}(\lambda)} \right.$$

$$\left. - \mathrm{Res}\,\{G_{N_s}(\lambda) = 0\} \right] \qquad (5.15)$$

where P, P' represent the distances from the defect in the lattice, and the contour C encloses all the poles of $P_{N_s N_b}^{-1}(\lambda)$, $G_{N_s}^{-1}(\lambda)$ but no others (Fig. 5.1)
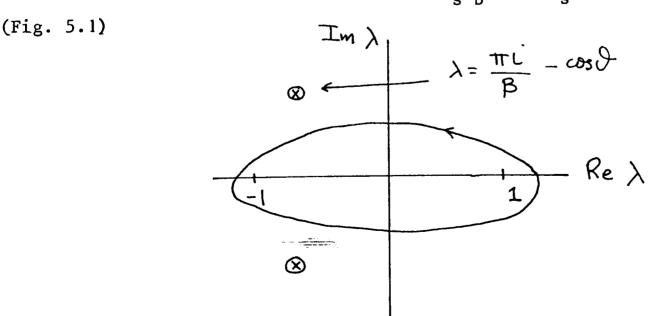

Figure 5.1. The complex λ plane with the contour C.

The limit $N_b \to \infty$ can now readily be established by using proposition (4.2). We have

$$F_1(t) = \frac{1}{2\pi} \int_0^{2\pi} d\theta \; e^{i(m-m')\theta} \; e^{-it\cos\theta} \; \frac{1}{2\pi i} \left[\oint_C \frac{e^{-it\lambda} G_{N_s}(p,\lambda) G_{N_s}(p',\lambda) d\lambda}{\beta(\cos\theta+\lambda)[1+e^{}] G_{N_s}(\lambda) P_{N_s\infty}(\lambda)} \right.$$

$$\left. - \text{Res} \{ G_{N_s}(\lambda) = 0 \} \right] \qquad (5.16)$$

where $P_{N_s\infty}(\lambda)$ is defined in (4.28) and the contour C is an ellipse on the Riemann sheet chosen by $(\lambda^2-1)^{\frac{1}{2}} > 0$, $\lambda > 0$. The following proposition establishes the limit, $t \to \infty$ for $F_1(t)$.

Proposition 5.1

$$\lim_{t\to\infty} F_1(t) = 0 \qquad (5.18)$$

Proof: There are two situations to be considered

$$\text{(i)} \quad \gamma^2 \le 1 + \frac{1}{N_s} \qquad \text{(ii)} \quad \gamma^2 > 1 + \frac{1}{N_s}$$

The properties of the function $P_{N_s,\infty}(\lambda)$ for these two regions are given in proposition (4.3). The contour C for the two regions enclose the cut from $[-1,1]$ and any isolated poles on the real line of the $(\lambda^2-1)^{\frac{1}{2}} > 0$, $\lambda > 0$ sheet. Using the residue theorem and the mapping $\lambda = \cos\psi$, the analysis proceeds along the same lines as that given in section 4, Chapter IV to give

$$F_1(t) = -\frac{1}{2\pi} \int_0^{2\pi} d\theta \; e^{i(m-m')\theta} \; e^{-it\cos\theta} \; \frac{1}{2\pi i} \int_{\Gamma'} \frac{e^{it\cos\psi} \cdot \sin(N_s-p)\psi \cdot \sin(N_s-p')\psi}{[1+e^{\beta(\cos\theta+\cos\psi)}] \cdot \sin N_s\psi}$$

$$\cdot \; \frac{d\psi}{\sin(N_s+1)\psi - \gamma^2 \cdot \sin N_s\psi \; e^{-i\psi}}$$

$$+ \delta(\gamma) \frac{1}{2\pi} \int_0^{2\pi} d\theta \ e^{i(m-m')\theta} \ e^{-it\cos\theta} V(\beta,\cos\theta,X_o) \qquad (5.19)$$

where Γ' is shown in Figure (4.4) and

$$\delta(\gamma) \ = \ \begin{array}{ll} 1 & \gamma^2 > 1 + {}^1/N_s \\ \\ 0 & \gamma^2 \leq 1 + {}^1/N_s \end{array}$$

$V(\beta,\cos\theta,X_o)$ corresponds to the residue obtained from the isolated

singularity of the functions $P_{N,\infty}(\cos\psi)$.

In the domain of integration the integrals in (5.19) satisfy the

Riemann-Lebesgue Lemmas and we conclude that $\underset{t\to\infty}{\text{Lim}} \ F_1(t) = 0$ //.

We remark here that the result (5.18) is true, independently of

the location of (n,m), (n'm'). In addition it is easily shown that it

remains true, for the limit sequence $M, N_b, N_s, t \to \infty$. Due to the dimension-

ality of the lattice Ω this result is true for all values of γ! The effect

of considering a lattice of one dimension is easily seen from (5.12) by

setting $M = 1$. In this case

$$F_1(t) \ = \ \sum_j \ T_{nj} T_{n'j} \ e^{-it\lambda_j} \ <X_j^\dagger X_j> \qquad (5.20)$$

and a study of the properties of $F_1(t)$ shows that

$$F_1(t) \ \underset{\sim}{\overset{t\to\infty}{}} \ 0(t^{-1}) \qquad \gamma^2 \leq 1 + \frac{1}{N_s}$$

$$\qquad (5.21)$$

$$F_1(t) \ \underset{\sim}{\overset{t\to\infty}{}} \ \text{Res.}(X_o)e^{itX_o} + \text{Res.}(-X_o)e^{-itX_o} \qquad \gamma^2 > 1 + \frac{1}{N_s}$$

where X_o is the frequency of the isolated eigenvalue.

To conclude this section we have shown that $A_{nm}, A_{n'm'}$ form a mixing

pair of local operators. In the case of the lattice of dimension $d = 2$

this is true for all values of the 'defect' strength γ, but only for $\gamma^2 \leq 1 + \frac{1}{N_s}$ for $d = 1$.

2. The Properties of the Relaxation Rate

As was remarked at the end of Chapter III, and briefly at the end of Chapter IV, two features of the behaviour of the system as it returned to the equilibrium, were striking.

(a) The rate at which equilibrium was attained was non-exponential.

(b) The relaxation rate depended on the size of the system Ω_s.

We shall now examine these two features in more detail, in the weak coupling limit. That is we rescale the time as

$$\tau = \gamma^2 t \qquad (5.22)$$

where we allow $\gamma^2 \to 0$, $t \to \infty$, τ is kept constant. The physical reasoning behind this special limiting procedure is that as we allow the coupling between the system and the heat bath to become weaker, we have to wait longer for the cumulative effect of the interaction to be observable.

We start with equation (4.34) which contains the time dependence of the initial state of Ω_s. For $\gamma^2 \neq 0$ we can use (4.13) to write

$$I(t) = \gamma^2 \sum_j \frac{e^{it\lambda_j}}{\lambda_j - \cos\phi_s} \cdot \frac{G_{N_s}(p,\lambda_j)G_{N_b}(\lambda_j)}{N^2(\lambda_j)} \qquad (5.23)$$

Writing this as a contour integral, and taking the limit $N_b \to \infty$ by the techniques described earlier we obtain

$$I(t) = \frac{\gamma^2}{2\pi i} \oint_C \frac{e^{it\lambda}}{\lambda - \cos\phi_s} \frac{G_{N_s}(p,\lambda)(\lambda - \sqrt{\lambda^2 - 1})d\lambda}{P_{N_s,\infty}(\lambda)} \qquad (5.24)$$

As the region of interest is for small γ^2, we shall certainly be inside the range $\gamma^2 < 1 + \frac{1}{N_s}$ (see proposition (4.3)) and the contour C encloses the cut in the complex λ plane between $[-1,1]$. Contacting the contour

onto the cut, (5.24) can be written

$$I(t) = \frac{\gamma^2}{\pi} \int_{-1}^{1} \frac{e^{it\lambda} G_{N_s}(p,\lambda)(1-\lambda^2)^{\frac{1}{2}} d\lambda}{(\lambda-\cos\phi_s) L(\gamma^2,\lambda)} \qquad (a)$$

$$\qquad (5.25)$$

$$L(\gamma^2,\lambda) = 1-\gamma^2 2\lambda G_{N_s}(\lambda) + \gamma^4 G_{N_s}^2(\lambda) \qquad (b)$$

with

$$G_{N_s}(p,\lambda) = \frac{U_{N-p-1}(\lambda)}{U_N(\lambda)} \qquad (5.26)$$

with the U's being Chebyshev polynomials of the 2nd kind.

Using (5.22) and defining a new variable

$$u = \frac{\lambda}{\gamma^2} \qquad (5.27)$$

we obtain

$$I(\tau) = \frac{\gamma^4}{\pi} \int_{-1/\gamma^2}^{1/\gamma^2} \frac{e^{i\tau u} G_{N_s}(p,\gamma^2 u)(1-\gamma^4 u^2)^{\frac{1}{2}} du}{(\gamma^2 u-\cos\phi_s)L(\gamma^2,\gamma^2 u)} \qquad (5.28)$$

Choosing N_s to be odd, using (5.26) and retaining only terms of order γ^2 (for N_s even, the lowest order terms are of order γ^4) we have

$$I(\tau) = \frac{1}{\pi} \int_{-1/\gamma^2}^{1/\gamma^2} \frac{e^{i\tau u}(C_1+C_2\gamma^2) du}{(N+1)^2 u^2 - 2\gamma^2 u^2(N+1) + 1} \qquad (5.29)$$

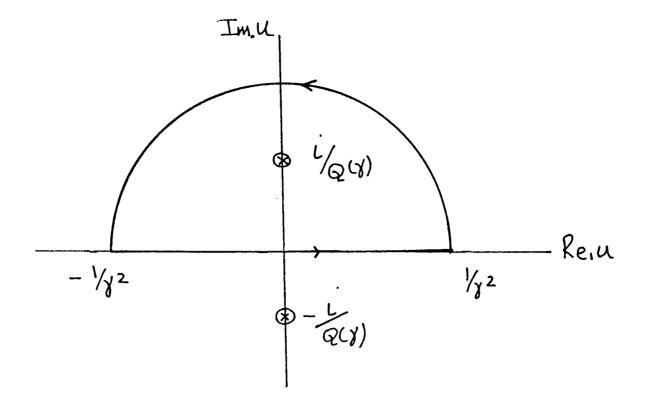where the values of C_1 and C_2 depend on ϕ_s, and P, and may be zero for some particular combinations of these.

Figure 5.3.

To analyse the behaviour of (5.29) we write

$$I(\tau) = \frac{1}{\pi} \oint_1 \frac{e^{i\tau u}(C_1 + C_2\gamma^2)du}{u^2 Q^2(\gamma) + 1} - \int_{\substack{semi-\\circle}} \frac{e^{i\tau u}(C_1 + C_2\gamma^2)du}{u^2 Q^2(\gamma) + 1}$$

(5.30)

where the contour 1 is illustrated in figure (5.3) and

$$Q^2(\gamma) = \{(N+1)^2 - 2\gamma^2(N+1)\}$$

(5.31)

Using the residue theorem, and calculating the contribution to the function $I(\tau)$ from the contour along the semicircular path, we obtain

$$I(\tau) = \frac{C_1 + C_2\gamma^2}{Q(\gamma)} e^{-\tau/Q(\gamma)} + \gamma^4 0(\tau^{-1})$$

(5.32)

We see that the decay to equilibrium in the <u>new</u> time scale is initially exponential, but is ultimately submerged in a non-exponential relaxation. However within the approximation of retaining terms to order γ^2 the second term in (5.32) may be dropped. In the limit $\gamma^2 \to 0$ $I(\tau)$ is

$$\underset{\gamma^2 \to 0}{\text{Lim}} \, I(\tau) = \frac{C_1}{N+1} e^{-\frac{\tau}{N+1}}$$

(5.33)

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The dependence of the relaxation rate on the size of Ω_S is clearly shown in (5.33). The <u>larger $|\Omega_S|$ the slower the rate</u> at which the system returns to equilibrium; the relaxation rate is <u>not</u> uniformly bounded in N_S. Introducing a new time scale, $\tau = (N_S+1)^{-1}\gamma^2 t$ removes this dependence, and results in a constant relaxation rate.

Analysis of $P(t)$, (4.43) which determines the time dependence of $|\Omega_B|$, the heat bath yields the same qualitative results.

3. <u>The Limit $N_S \to \infty$</u>.

In this section we examine the behaviour of $<f^\dagger_{nm} f_{nm}>_t$ when both N_S, and N_b are allowed to approach infinity. The following propositions give the spectral properties of $H(\Omega)$, the Hamiltonian for the whole lattice.

<u>Proposition 5.1</u>

The limit of the polynomial P_{N_S,N_b}, when N_S, $N_b \to \infty$ is given by

$$P_\infty(\lambda) = 1-\gamma^2(\lambda - \sqrt{\lambda^2-1})^2 \tag{5.34}$$

with choice of branch $(\lambda^2-1)^{\frac{1}{2}} > 0$; $\lambda > 0$.

<u>Proof</u>: This follows immediately from proposition (4.2) by taking the limit $N_S \to \infty$ in (4.28).//

<u>Proposition 5.2</u>

The spectrum of $H(\Omega)$ is continuous and bounded for $\gamma^2 \leq 1$ and is represented by the cut $[-1,1]$ in the complex λ plane. For $\gamma^2 > 1$ the spectrum consists of a continuous part (the cut from $[-1,1]$) and two isolated eigenvalues represented by the zeroes of (5.34) in the Riemann sheet defined by $(\lambda^2-1)^{\frac{1}{2}} > 0$, $\lambda > 0$.

<u>Proof</u>: It is readily verified that $P_\infty(\lambda)$ has roots $\lambda = \pm \frac{1}{2}(\gamma + \frac{1}{\gamma})$, moreover the region $\gamma^2 < 1$ corresponds to the choice of branch $(\gamma^2-1)^{\frac{1}{2}} < 0$ for $\lambda > 0$, so that the roots which lie on this Riemann sheet may be ignored. For $\gamma^2 > 1$ the roots lie on the sheet defined by $(\lambda^2-1)^{\frac{1}{2}} > 0$, $\lambda > 0$ and these will correspond to the isolated eigenvalues.//

To examine the behaviour of $<f_{nm}^{\dagger}f_{nm}>_t$ near the boundary we put

$p = 0$, that is $n = N_s$ in equations (4.23) and (4.24) to obtain

$$<f_{nm}^{\dagger}f_{nm}>_t = S(\beta_1,t,\gamma) + B(\beta_2,t,\gamma) \tag{5.35}$$

where

$$S(\beta_1,t,\gamma) = \frac{1}{M(N_s+1)} \sum_{1,s} \frac{2\sin^2\phi_s}{1+e^{\beta_1(\cos\phi_s+\cos\theta_1)}} \left| \sum_j \frac{e^{it\lambda_j}}{\lambda_j-\cos\phi_s} \cdot \frac{1}{N^2(\lambda_j)} \right|^2 \tag{5.36}$$

$$B(\beta_2,t,\gamma) = \frac{1}{M(N_b+1)} \sum_{1,b} \frac{2\sin^2\phi_b}{1+e^{\beta_2(\cos\phi_b+\cos\theta_1)}} \left| \sum_j \frac{\gamma e^{it\lambda_j}}{\lambda_j-\cos\phi_b} \cdot \frac{G_{N_s}(\lambda_j)}{N^2(\lambda_j)} \right|^2 \tag{5.37}$$

The limits $M,N_s,N_b \to \infty$ may now be obtained by following the procedures

described in section 3 of Chapter IV. We obtain for (5.36) and (5.37)

$$S(\beta,t,\gamma) = \frac{1}{4\pi^2} \int_0^{2\pi} d\theta \int_{-\pi}^{\pi} d\phi \frac{2\sin^2\phi}{1+e^{\beta_1(\cos\theta+\cos\phi)}} \cdot \frac{1}{2\pi i} \oint_C \frac{e^{it\lambda}}{(\lambda-\cos\phi)} \cdot \frac{d\lambda}{P_\infty(\lambda)} \tag{5.38}$$

$$\cdot \frac{1}{2\pi i} \oint_C \frac{e^{-it\lambda}}{\lambda-\cos\phi} \frac{d\lambda}{P_\infty(\lambda)}$$

$$B(\beta_2,t,\gamma) = \frac{1}{4\pi^2} \int_0^{2\pi} d\theta \int_{-\pi}^{\pi} d\phi \frac{2\sin^2\phi}{1+e^{\beta_2(\cos\theta+\cos\phi)}} \cdot \frac{\gamma}{2\pi i} \oint_C \frac{e^{it\lambda}}{\lambda-\cos\phi} \frac{(\lambda-\sqrt{\lambda^2-1})\,d\lambda}{P_\infty(\lambda)} \tag{5.39}$$

$$\cdot \frac{\gamma}{2\pi i} \oint_C \frac{e^{-it\lambda}(\lambda - \sqrt{\lambda^2-1})\,d\lambda}{(\lambda-\cos\phi)\,P_\infty(\lambda)}$$

The contours C lie on the Riemann sheet defined by $(\lambda^2-1)^{\frac{1}{2}} > 0$, $\lambda > 0$ and enclose the cut, and any isolated real poles on this sheet. To analyse the time dependence we shall examine the two integrals

$$X(t) = \frac{1}{2\pi i} \oint_C \frac{e^{it\lambda} \, d\lambda \, \sin\phi}{(\lambda - \cos\phi) P_\infty(\lambda)} \qquad (5.40)$$

$$X(t) = \frac{1}{2\pi i} \oint_C \frac{e^{it\lambda} \, (\lambda - \sqrt{\lambda^2-1}) \, d\lambda \cdot \sin\phi}{(\lambda - \cos\phi) \, P_\infty(\lambda)} \qquad (5.41)$$

Making the substitution $\lambda = \cos\psi$, and noting that both integrands have the same denominator we have

$$X(t) = \frac{-1}{2\pi i} \int_{\Gamma^-} \frac{e^{it\cos\psi} \sin\phi \cdot \sin\psi \cdot d\psi}{(\cos\psi - \cos\phi) \{1 - \gamma^2 e^{-i2\psi}\}} \qquad (5.42)$$

$$Y(t) = \frac{-1}{2\pi i} \int_{\Gamma^-} \frac{e^{it\cos\psi} \sin\phi e^{-i\psi} \cdot \sin\psi \cdot d\psi}{(\cos\psi - \cos\phi) \{1 - \gamma^2 e^{-i2\psi}\}} \qquad (5.43)$$
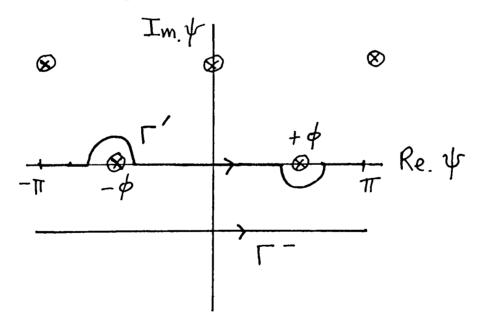

Figure 5.4. Complex ψ plane

Where the transformation maps on elliptical contour C in the λ plane to Γ^- in the ψ plane. The region $\text{Im}\psi \; \epsilon[0,-\infty]$, $\text{Re}\psi \; \epsilon[-\pi,\pi]$ corresponds to the $(\lambda^2-1)^{\frac{1}{2}} > 0$, $\lambda > 0$ Riemann sheet and $\text{Im}\psi \; \epsilon[0,\infty]$ $\text{Re}\psi \; \epsilon[-\pi,\pi]$ to the $(\lambda^2-1)^{\frac{1}{2}} < 0$, $\lambda > 0$ Riemann sheet. From proposition (5.2) we conclude

that the zeroes of $1 - \gamma^2 e^{-i2\psi}$ will lie in the top half of the ψ plane

for $\gamma^2 > 1$ and in the lower half of the plane for $\gamma^2 < 1$. Using the

periodic properties of the integrands we can write

$$X(t) = \frac{e^{itcos\phi} \cdot sin\phi}{1 - \gamma^2 e^{+i2\phi}} - \frac{1}{2\pi i} \int_{\Gamma^-} \frac{e^{itcos\psi} \cdot sin\phi \cdot sin\psi \cdot d\psi}{(cos\psi - cos\phi)\{1 - \gamma^2 e^{-i2\psi}\}}$$

(5.44)

$$Y(t) = \frac{e^{itcos\phi} e^{i\phi} \cdot sin\phi}{(1 - \gamma^2 e^{+i2\phi})} - \frac{1}{2\pi i} \int_{\Gamma^-} \frac{e^{itcos\psi} \cdot sin\phi \, e^{-i\psi} \cdot sin\psi \cdot d\psi}{(cos\psi - cos\phi)\{1 - \gamma^2 e^{-i2\psi}\}}$$

(5.45)

where we restricted our attention to the region $\gamma^2 \leq 1$. For $\gamma^2 > 1$ we

obtain an additional oscillating term due to the presence of the isolated

eigenvalues. For large times the integrals along Γ' tend to zero, and

so we obtain, using (5.45) and (5.46) in (5.38), (5.39)

$$\begin{array}{c} \text{Lim.} \\ M, N_s, N_b \to \infty \\ t \to \infty \\ \gamma^2 \leq 1 \end{array} <f_{N_s m}^{\dagger} f_{N_s m}>_t = \frac{1}{4\pi^2} \int_0^{2\pi} d\theta \int_{-\pi}^{\pi} d\phi \frac{2sin^2\phi}{(1+e^{\beta_1(cos\theta+cos\phi)})(1 - \gamma^2 2cos2\phi + \gamma^4)} \cdot$$

(5.46)

$$+ \frac{1}{4\pi^2} \int_0^{2\pi} d\theta \int_{-\pi}^{\pi} d\phi \frac{\gamma^2 2sin^2\phi}{(1+e^{\beta_2(cos\theta+cos\phi)})(1 - \gamma^2 2cos2\phi + \gamma^4)}$$

From (5.46) we seen that $|\Omega_S|$, $|\Omega_B| \to \infty$ first, and then $t \to \infty$ we obtain

contributions from both terms in (5.35), that is $<f_{N_s m}^{\dagger} f_{N_s m}>_t$ retains the

memory that at $t = 0$ it was in a state of inverse temperature β_1. This can

be understood in terms of the earlier discussion on the dependence of the

relaxation rate on the size of $|\Omega_S|$; equation (5.33) in particular shows

that in the weak coupling limit the relaxation rate is inversely propor-

tional to the length of Ω_S.

One might hope that in this limiting procedure, ie Ω_S, $\Omega_B \to \infty$

together, the time evolution of $<f^{\dagger}_{N_s m} f_{nm}>_t$ near the interaction boundary

might mimic the behaviour of a calorimeter. If this were the case we

would expect to obtain for the final state

$$\underset{\substack{(\Omega_S,\Omega_B) \to \infty \\ t \to \infty}}{\text{Lim}} <f^{\dagger}_{N_s m} f_{N_s m}>_t = <f^{\dagger}_{N_s m} f_{N_s m}>_{\frac{1}{2}(\frac{\beta_1 \beta_2}{\beta_1 + \beta_2})} \qquad (5.47)$$

We first note that we obtain the same answer in equation (5.46)

whether the limits Ω_S, $\Omega_B \to \infty$ are taken together or sequentially. This

can be readily seen if one examines the structure of equations (4.23) and

(4.24). Clearly the hope that the lattice Ω would behave as a calorimeter

is not realised, for (5.46) is not of the form (5.47). Moreover the separa-

tion of the motion $<f^{\dagger}_{nm} f'_{nm}>_t$ into two terms, as in (5.35), each of which

depends only on β_1, or β_2, makes the kind of result (5.47) impossible.

This situation is to be understood as follows: As long as Ω_S is.

finite, the overall equilibrium state is determined by the infinite part

of the lattice ie Ω_B, and in the limit $t \to \infty$ the finite region Ω_S will

return to the equilibrium state of Ω_B. In this sense the state of Ω_S is a

local deviation from the equilibrium state of Ω_B. When $|\Omega_S| \to \infty$ the two

parts of the lattice $\Omega = \Omega_S \cup \Omega_B$ make 'equal' contributions, the new

equilibrium state being at an intermediate temperature to that of either

Ω_S or Ω_B. Equations (5.46) and (5.47) show that (1.24) is not satisfied.

Under the time evolution generated by $H(\Omega)$ the lattice fails to approach

this new intermediate equilibrium state.

These results show that testing the time evolution for mixing proper-

ties, that is equation (1.25), the result will not give an indication as

to the validity of (1.24). Thus mixing is an insufficiently strong condition (at least for this model) to describe the kind of approach to equilibrium phenomena observed in real physical systems.

4. Concluding Remarks

The purpose of this section is to summarise the main results obtained for the model described in Chapter II, and place them in context of the discussion in Chapter I. The validity of equation (1.24) was examined by exact calculation of the equations of motion for the following two cases.

(i) The initial non-equilibrium state π given by

$$\pi \equiv \rho(0) = e^{-\beta_1 H(\Omega_S)} \otimes e^{-\beta_2 H(\Omega_B)} \tag{5.48}$$

with Ω_S finite, representing the observed system, and Ω_B infinite, representing a heat bath for Ω_S.

(ii) The initial state is given as in (5.48), but now Ω_S, and Ω_B are treated on an equal basis. Physically this would correspond to a calorimeter experiment, where the total lattice $\Omega = \Omega_S \cup \Omega_B$ is isolated, from the surroundings, and ultimately attains a new intermediate equilibrium state.

The results of this study show that in case (i) equation (1.24) is satisfied, that is the model mimics the behaviour of a real system, when this is coupled to a heat bath. The validity of (1.24) is subject to the requirement that the spectrum of the Hamiltonian generating the time evolution does not have any isolated eigenvalues. This is in accord with the results obtained for other 'harmonic' models as discussed in section 3 of Chapter I. The behaviour of these models, and the characterisation of the flow of classical systems in phase space in terms of the spectral properties of the Liouville operator, is very suggestive; in both cases isolated eigenvalues play an inhibiting role to ergodicity/mixing.

One curious feature of this model is that the relaxation rate

depends on the size of the system Ω_S. This is clearly exhibited when we study the time dependence in the weak coupling limit. Here we find that the non-exponential decay to equilibrium observed in the case of arbitrary coupling strength γ, becomes exponential in the new time scale $\tau(\tau = \gamma^2 t,\ t \rightarrow \infty,\ \gamma^2 \rightarrow 0, \tau$ fixed) with a relaxation rate inversely proportional to the size of Ω_S.

The Hamiltonian generating the time evolution is found to have mixing properties in the sense of equation (1.25), that is localised measurements made at different times, become statistically independent as the time interval separating them becomes very large. This means that as a result of the motion of the particles on the lattice, the effect of the first local measurement on the system, becomes dissipated throughout the infinite system, and so does not interfere with the second measurement. This is equivalent to saying that local perturbations will not effect the equilibrium state of the infinite lattice and will ultimately die away. In this sense the effect of the finite system Ω_S on the infinite Ω_B, may be considered as a local perturbation.

In the second case (ii), equation (1.24) _fails_ to be satisfied. The equilibrium state obtained by the action of the equations of motion on the non-equilibrium state (5.48) is not the expected _intermediate_ temperature state. This shows that the model does not mimic calorimetric behaviour observed in real systems, and does not describe the problem of how an isolated system approaches its equilibrium. Evidently mixing is not a sufficiently strong condition on the time evolution to describe this kind of behaviour.

* This chapter consists mostly of a
reproduction of Felderhof's (29)
calculations. The variation consists
in introducing the vectors $|\Phi_L\rangle$ in
(6.67) from which considerable
 simplifications result.

CHAPTER VI: SPIN RELAXATION IN THE ISING MODEL *

The time dependent statistics of the one dimensional Ising model [26] were first studied in an exact manner by Glauber [27]. A system described by the Ising model cannot change its state spontaneously as the spin operators σ_j^z commute with the Hamiltonian. In order that we obtain a dynamic model, an external agency, such as a heat bath is considered. The effect of this agency is to cause spontaneous flips of the spins in the Ising chain. This external heat bath does not enter the problem explicitly, but its presence is felt through <u>local</u> transition rates, defined through the rules of the model. The local transition rates give the rate per unit time at which a spin at site j will flip to a state of opposite spin value. In the case of the Glauber model, these transition rates are chosen to depend on the spin states of the nearest neighbours, and are supposed not to depend on the previous history of the system.

Time evolution in these stochastic models is defined through a master equation [28]. In this approach the system is described by a probability function P, and one must be given a stochastic operator T, in terms of which the time evolution is obtained through the linear equation

$$\frac{\partial P}{\partial t} = T \, P$$

The operator T is constructed directly from the local transition rates.

The problem of obtaining the spectrum of the stochastic operator with Glauber transition rates was solved by Felderhof [29] using techniques presented by Schultz et al [30] in their calculation of the partition function of the two dimensional Ising model. We show that by careful analysis of this method, it is possible to provide a simpler alternative to the Felderhof method for evaluating matrix elements encountered in studying the spin time dependence.

In Section 1 the relevant theoretical background is introduced,

followed in Section 2 by a brief introduction of the model and the modified calculation.

1. The Time Evolution

We consider a system to be characterised by a finite orthonormal set of states $\{|\psi_n> \ n = 1, \ldots N\}$ and an associated Hamiltonian H, such that

$$H|\psi_n> = E_n|\psi_n>; \quad <\psi_n|\psi_{n'}> = \delta_{nn'} \quad (6.1)$$

where E_n is the eigenvalue of the state $|\psi_n>$. A general state of the system will be described by

$$|\phi(t)> = \sum_n P_n(t) \ |\psi_n> \quad (6.2)$$

where the $P_n(t)$ are relative probabilities of being in the state $|\psi_n>$ at time t, and satisfy

$$\sum_n P_n(t) = 1 \quad (6.3)$$

The time evolution of the state vector $|\phi(t)>$, is defined through the Master equation [26]

$$\frac{\partial P_n(t)}{\partial t} = \sum_{m \neq n} \Big(w(n,m) \ P_m(t) - w(m,n) \ P_n(t) \Big) \quad (6.4)$$

which describes the time development of the probabilities $P_n(t)$. The first term of (6.4) represents the gain in probability from the other states $|\psi_m>$, and the second term of the rate of loss to the other states. The elements $w(n,m)$ represent the _transition rates_ between the states (n,m), and are positive or zero

$$w(n,m) \geq 0 \quad (6.5)$$

The time development of $|\phi(t)>$ is now given by

$$\frac{\partial|\phi(t)>}{\partial t} = T \ |\phi(t)> \quad (6.6)$$

* Equation (6.11) is actually
used for all operators but we
are only interested in operators
which are diagonal at time zero.

which defines the stochastic operator T. The matrix elements $T_{nm} = \langle\psi_n|T|\psi_m\rangle$ may now be determined from (6.4) and (6.2)

$$T_{nm} = w(n,m) \quad n \neq m \qquad (6.7)$$

$$T_{nn} = -\sum_{m \neq n} w(m,n) \qquad (6.8)$$

Equations (6.7) and (6.8) represent the conservation of probability flow as expressed in (6.4) and (6.3). This has the important consequence that the unit state $|1\rangle$

$$|1\rangle = \sum_n |\psi_n\rangle \qquad (6.9)$$

is a left eigenvector of the operator T with eigenvalue zero

$$\langle 1| \, T = 0 \qquad (6.10)$$

Time dependent averages of operators __diagonal__ in the $|\psi_n\rangle$ representation A are given by *

$$\langle A\rangle_t = \langle 1| \, A \, |\phi(t)\rangle \qquad (6.11)$$

For stochastic operators independent of time (6.6) may be integrated to yield

$$\langle A\rangle_t = \langle 1| \, A \, e^{tT} \, |\phi_o\rangle \qquad (6.12)$$

where $|\phi_o\rangle$ is an initial state of the system. Equation (6.10) allows us to define a 'Heisenberg' type evolution for the operator $A(t)$

$$A(t) = e^{-tT} A(0) \, e^{tT} \qquad (6.13)$$

The time delayed correlation functions may now be evaluated from

$$\langle A(t) \, B(0)\rangle = \langle 1| \, A(t) \, B(0) \, |\phi_o\rangle \qquad (6.14)$$

where A, B are operators diagonal in the $|\psi_n\rangle$ representation.

Equation (6.10) shows that zero is an element of the spectrum of the

operator T. From (6.6) we therefore associate the equilibrium state to be a right eigenvector

$$T \; |\phi_e> \; = \; 0 \tag{6.15}$$

with $|\phi_e>$ the equilibrium state. At equilibrium the detailed balance condition is satisfied . **This is a hypothesis postulated on physical grounds.**

$$w(n,m) \; P_m(eq.) \; = \; w(m,n) \; P_n(eq.) \tag{6.16}$$

The equilibrium state is chosen by requiring that $P_n(eq.)$ be of the form

$$P_n(eq.) \; = \; e^{-\beta E_n} \tag{6.17}$$

where E_n is given in (6.1). From (6.16) the symmetry relation

$$e^{\beta/2 E_n} \; w(n,m) \; e^{-\beta/2 E_m} \; = \; e^{\beta/2 E_m} \; w(m,n) \; e^{-\beta/2 E_n} \tag{6.18}$$

provides a way of symmetrising the operator T through the similarity transform

$$T(\beta) \; = \; e^{+\beta/2 H} \; T \; e^{-\beta/2 H} \tag{6.19}$$

This ensures that (6.17) is satisfied.

Theorem 6.1

The spectrum of the operator $T(\beta)$ is (i) Real; (ii) is contained in the interval $(-\infty, 0]$.

Proof:

(i) From (6.18) it follows that $T_{nm}(\beta) = T_{mn}(\beta)$, thus $T(\beta)$ is a symmetric operator. This establishes the reality of the spectrum.

(ii) We prove this by showing that $T(\beta)$ is negative semi-definite [31]. The matrix elements of $T(\beta)$ are

$$T_{nm}(\beta) \; = \; (1 - \delta_{mn}) \; P_n^{\frac{1}{2}}(eq.) \; w(n,m) \; P_m^{\frac{1}{2}}(eq.)$$

$$- \delta_{nm} \sum_{r \neq n} w(r,n) \qquad (6.20)$$

Forming the function G(Y)

$$G(Y) = \sum_{n,m} Y_n T_{nm} Y_m \qquad (6.21)$$

we find

$$G(Y) = - \sum_{\substack{r,n \\ r \neq n}} w(r,n) Y_n^2 + \sum_{\substack{n,m \\ n \neq m}} w(n,m) P_n^{\frac{1}{2}}(eq.) P_m^{\frac{1}{2}}(eq.) Y_n Y_m$$

$$= - \frac{1}{2} \sum_{n,m} w(n,m) \overset{P_n(eq.)}{P_m(eq.)} \left[\frac{Y_n}{P_n^{\frac{1}{2}}(eq.)} - \frac{Y_m}{P_m^{\frac{1}{2}}(eq.)} \right]^2 \qquad (6.22)$$

Equation (6.5), (6.17) show that $G(Y) \leq 0$ for all Y showing that $T(\beta)$ is negative semi-definite.//

2. **Spin Relaxation in the Ising Model**

Consider a one-dimensional spin system on a lattice Ω, interacting via the Ising Hamiltonian

$$H(\Omega) = - J \sum_{j \in \Omega} \sigma_j^z \sigma_{j+1}^z \qquad (6.23)$$

where $J > 0$ is the interaction parameter. The basic states of the system $|\psi_n\rangle$ are constructed from the spin states $|\mu\rangle$

$$|\mu\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{if } \mu = +1$$

$$(6.24)$$

$$|\mu\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad \text{if } \mu = -1$$

with

$$\sigma^z |\mu\rangle = \mu |\mu\rangle \qquad (6.25)$$

where σ^z, σ^y, σ^x are the Pauli spin operators and satisfy

$$[\sigma^x, \sigma^y]_- = 2i \, \sigma^z \qquad (6.26)$$

Thus the 2^N possible states $|\psi_n\rangle$ are of the form

$$|\psi_n\rangle = |\mu_1\rangle \, |\mu_2\rangle \, \cdots \, |\mu_N\rangle = |\mu_1, \mu_2, \mu_3, \, \cdots \, , \mu_N\rangle \qquad (6.27)$$

and operators σ_j^z acting in the 2^N dimensional state space of the spin system, are given by the direct product

$$\sigma_j^z = \overset{j-1}{\underset{i=1}{\bigotimes}} \; I \otimes \sigma^z \; \overset{N}{\underset{i=j+1}{\bigotimes}} \; I \qquad (6.28)$$

so that

$$\sigma_j^z \, |\psi_n\rangle = \mu_j \, |\psi_n\rangle \qquad (6.29)$$

Operators σ_j^x, σ_j^y are similarly defined. That the states $|\psi_n\rangle$ are orthonormal follows from the properties of $|\mu\rangle$ as defined in (6.24). The transition rates that a spin at site j, of the chain changes state from $|\mu_j\rangle$ to $|-\mu_j\rangle$, were formulated by Glauber [27] to be of the form

$$W(n,n') = \sum_{j=1}^{N} \frac{1}{2} \{ 1 - \frac{\gamma}{2} \mu_j (\mu_{j-1} + \mu_{j+1}) \} \prod_{k \neq j} \delta_{\mu_k \mu_k'} \, \delta_{|\mu_j - \mu_j'|, 2}$$

$$(6.30)$$

where the Kronecker deltas ensure that only one spin changes at any one instant in time. In principle it is possible to choose an infinite variety of transition rates, the special feature of Glauber's choice is that it leads to a tractable problem where the exact solutions may be obtained.

Consider the effect of the operator σ_j^x on a state $|\psi_n\rangle$

$$\sigma_j^x \, |\mu_1, \, \cdots \, , \mu_j, \, \cdots \, , \mu_N\rangle = |\mu_1, \, \cdots \, , -\mu_j, \, \cdots \, \mu_N\rangle \qquad (6.31)$$

It thus generates the state that differs from $|\psi_n\rangle$ in that the spin at the jth site has opposite spin configuration. Using (6.31), (6.30), (6.7), (6.8) it is possible to construct the spin representative of the stochastic operator as

$$T = \frac{1}{2} \sum_{j=1}^{N} [(1 + \frac{\gamma}{2} \sigma_j^z(\sigma_{j-1}^z + \sigma_{j+1}^z)) \sigma_j^x - 1 + \frac{\gamma}{2} \sigma_j^z(\sigma_{j+1}^z + \sigma_{j-1}^z)]$$

(6.32)

where cyclic boundary conditions are employed

$$\sigma_{n+j}^1 = \sigma_j^1 \quad (1 = x,y,z)$$

(6.33)

From the detailed balance condition (6.16), and equilibrium states of the Ising Hamiltonian, the parameter γ satisfies

$$\gamma = \text{th}2V \quad (V = \beta J)$$

(6.34)

The non-hermitian operator T in (6.32), may be symmetrised through the similarity transform (6.19). We find

$$\mathcal{T}(V) = \frac{1}{2} \sum_{j=1}^{N} [(\cos^2\theta - \sigma_{j-1}^z\sigma_{j+1}^z \sin^2\theta)\sigma_j^x - 1 + \frac{\gamma}{2} \sigma_j^z(\sigma_{j-1}^z + \sigma_{j+1}^z)]$$

(6.35)

where

$$\sin\theta = \text{ShV}/(\text{Ch}2V)^{\frac{1}{2}}$$

$$\cos\theta = \text{ChV}/(\text{Ch}2V)^{\frac{1}{2}}$$

(6.36)

$$\gamma = \sin^2\theta$$

and the angle $\theta\epsilon(0,^\pi/4)$. To obtain the diagonal form of the operator (6.35), we employ its translational symmetry

$$C \sigma_j^z C^{-1} = \sigma_{j-1}^z$$

(6.37)

where C is a translation operator, which generates the cyclic group C_N. To exploit this symmetry, we introduce the Jordan-Wigner transformation [32]

$$f_n^\dagger = \prod_1^{n-1} (\sigma_j^{\ x}) \frac{1}{2}(\sigma_n^{\ z} + i\sigma_n^{\ y}) \qquad (6.38)$$

$$f_n = \prod_1^{n-1} (\sigma_j^{\ x}) \frac{1}{2}(\sigma_n^{\ z} - i\sigma_n^{\ y}) \qquad (6.39)$$

which defines fermion creation/annihilation operators $f_n^\dagger$, f_n, satisfying the anticommutation rules (2.3). These operators have the advantage that the anticommutator algebra is preserved under unitary transformations. The spin operators $\sigma_j^{\ l}$ (l = x,y,z) are given in terms of the fermion operators by

$$\sigma_n^{\ x} = (1 - 2f_n^\dagger f_n)$$

$$\sigma_n^{\ y} = -i \prod_1^{n-1} (\sigma_j^{\ x})(f_n^\dagger - f_n) \qquad (6.40)$$

$$\sigma_n^{\ z} = \prod_1^{n-1} (\sigma_j^{\ x})(f_n^\dagger + f_n)$$

The stochastic operator $T(V)$ expressed in terms of fermion operators, acts in the state space h of dimension 2^N, and the new set of vectors

$$|0>, \ f_j^\dagger \ |0>, \ f_j^\dagger \ f_1^\dagger \ |0>, \ \ldots \qquad (6.41)$$

are a basis for this state space. The vacuum state $|0>$ is defined to be the state

$$f_j \ |0> = 0 \qquad (6.42)$$

for all j, and it may be readily identified with

$$|0\rangle \equiv |1\rangle = \binom{1}{1}_1 \binom{1}{1}_2 \binom{1}{1}_3 \cdots \binom{1}{1}_N \tag{6.43}$$

Using (6.40), and making the observation that the fermion operators occur in pairs, it is seen that $T(V)$ commutes with the parity operator

$$U = \prod_1^N e^{\pi i\, f_j^\dagger f_j} \tag{6.44}$$

and its states can be classified according to their parity. Further with the choice

$$f_{N+j} = -f_j \quad \text{for} + \text{parity states}$$

$$f_{N+j} = f_j \quad \text{for} - \text{parity states} \quad , \tag{6.45}$$

the operator $T(V)$ can be written as

$$T(V) = T^+(V)P_+ + T^-(V)P_- \tag{6.46}$$

where

$$P_\pm = \frac{1}{2}(I \pm U) \tag{6.47}$$

are projectors onto +/- parity states, and

$$T^\pm(V) = \frac{1}{2}\sum_1^N [\cos^2\theta\ (1 - 2f_j^\dagger f_j) - \sin^2\theta\ (f_{j-1}^\dagger - f_{j-1})(f_{j+1}^\dagger + f_{j+1})$$

$$- 1 + \gamma\ (f_j^\dagger - f_j)(f_{j+1}^\dagger + f_{j+1})] \tag{6.48}$$

the $\pm$ refer to the appropriate boundary conditions (6.45). The operators $T^\pm$ (V) thus act in the corresponding even/odd subspaces of h

$$h = h_+ \oplus h_- \tag{6.49}$$

Use of the translational symmetry is now made by defining new fermion operators, via the spatial Fourier transform

$$F_k^\dagger = N^{-\frac{1}{2}} \sum_n e^{ikn} f_n^\dagger \qquad (6.50)$$

The allowed k values obtained by imposing the boundary conditions (6.45) can be classed into two sets $S^{\pm}$

$$S^{\pm} = \{e^{ikn} = \mp 1\} \qquad (6.51)$$

the elements of each set, given by the roots of the appropriate equation. In terms of these new fermion operators the operators $T^{\pm}$ take the form

$$T^{\pm}(V) = \sum_{k \in S^{\pm}} T_k(V) \qquad (6.52)$$

$$T_k(V) = -[C_k(F_k^\dagger F_k + F_{-k}^\dagger F_{-k} - 1) - i D_k(F_k^\dagger F_{-k}^\dagger + F_k F_{-k}) + 1] \qquad (6.53)$$

$C_k = \cos^2\theta + \sin^2\theta \cdot \cos 2k - \gamma\cos k$

$D_k = -\sin^2\theta \cdot \sin 2k + \gamma\sin k$

From (6.51) we denote the elements of the sets $S^{\pm}$ by $\{\beta\}$, $\{\alpha\}$ respectively, and each of the operators $T^{\pm}$ acts in the state space generated by the complete basis sets

$$h_\beta : \{|0>, F_\beta^\dagger |0>, F_{\beta_1}^\dagger F_{\beta_2}^\dagger |0>, \ldots \} \quad \text{for } T^+(V)$$

$$\qquad (6.54)$$

$$h_\alpha : \{|0>, F_\alpha^\dagger |0>, F_{\alpha_1}^\dagger F_{\alpha_2}^\dagger |0>, \ldots \} \quad \text{for } T^-(V)$$

From (6.46) the projectors P_+ allow only the even/odd parity states of h_β/h_α. The operators $F_\beta^\dagger$, and $\bar{F}_\alpha^\dagger$ are connected by a transformation function $<\beta|\alpha>$

$$<\beta|\alpha> = 2[N(e^{i(\beta-\alpha)} - 1)]^{-1} \qquad (6.55)$$

$$F_\alpha^\dagger = \sum_\beta F_\beta^\dagger <\beta|\alpha> \qquad (6.56)$$

Moreover these sets of operators satisfy Fermi anticommutation rules

$$[F_k^\dagger, F_{k'}]_+ = \delta_{kk'} \quad [F_k, F_{k'}]_+ = 0 \qquad (6.57)$$

if both $k, k' \in S^+$ or S^-, but

$$[F_\beta^\dagger, F_\alpha]_+ = \langle \alpha | \beta \rangle \qquad (6.58)$$

Canonicality is preserved if both k, k' are in the same class $S^{\pm}$.

To complete the diagonalisation of the operator (6.53) a new set of fermion operators is introduced by [33]

$$G_k^\dagger = \cos\omega(k) F_k^\dagger - i \sin\omega(k) F_{-k} \qquad (6.59)$$

$$e^{\pm i\omega(k)} (G_k^\dagger \pm G_{-k}) = F_k^\dagger \pm F_{-k} \qquad (6.60)$$

$k = \{\beta, \text{ or } \alpha\}$. Canonicality of operators in the same class is assured since $\omega(k) = -\omega(-k)$ (mod. π). The transformation angle $\omega(k)$ is obtained, through the condition that the new fermion operators satisfy

$$[T_k(V), G_k^\dagger]_- = \lambda_k G_k^\dagger \qquad (6.61)$$

Solving for λ_k, and $\omega(k)$ we obtain

$$\lambda_k = 1 - \gamma \cos k \qquad (6.62)$$

$$\tan \omega(k) = \frac{\sin\theta . \sin k}{\sin\theta . \cos k - \cos\theta} \qquad (6.63)$$

It is useful to define here the function Θ (e^{ik}) as

$$\Theta (e^{ik}) = e^{-i2\omega(k)} \qquad (6.64)\cdot$$

and for the particular case (6.63)

$$\Theta \ (e^{ik}) \ = \ e^{-ik} \ \{\frac{\tan\theta \ - \ e^{ik}}{e^{ik}\tan\theta- \ 1}\} \tag{6.65}$$

The relation (6.63) for the transformation angle $\omega(k)$ is well defined for all $k\epsilon S^{\pm}$ in the domain $\theta\epsilon[0,^{\pi}/4)$. The point $\theta = {}^{\pi}/4$ corresponds to the system at zero temperature, further $\omega(0) = \omega(\pi) = 0$ except at zero temperature.

The new operators $G_k^{\dagger}$ diagonalise T_k

$$T_k(V) \ = \ - \ \frac{1}{2} \ \{\lambda_k \ (2G_k^{\dagger}G_k \ -1) \ +1\} \tag{6.66}$$

To obtain the new vacua for the operators G_k we note that they must be proportional to $G_kG_{-k}|0>$. Using (6.59) it is readily verified that

$$|\Phi_{\pm}> \ = \ \prod_{k\epsilon S^{\pm}} \ (\cos \ \omega(k) \ + \ i \ \sin \ \omega(k) \ F_{-k}^{\dagger}F_k^{\dagger}) \ |0> \tag{6.67}$$

where

$$G_{\beta} \ |\Phi_+> \ = \ G_{\alpha} \ |\Phi_-> \ = \ 0 \tag{6.68}$$

for all $\{\beta\}$, $\{\alpha\}$. The allowed states of the system are given as

(i) + parity states: $|\Phi_+>, \ G_{\beta_1}^{\dagger} G_{\beta_2}^{\dagger} \ |\Phi_+>, \ ...$ $\tag{6.69}$

(ii) - parity states: $G_{\alpha}^{\dagger} \ |\Phi_->, \ G_{\alpha_1}^{\dagger} G_{\alpha_2}^{\dagger} G_{\alpha_3}^{\dagger} \ |\Phi_-> \ ...$ $\tag{6.70}$

The state $|\Phi_+>$ corresponds to the zero eigenvalue of the operator $T(V)$

$$T(V) \ = \ \{- \ \frac{1}{2} \ \sum_{\beta\epsilon S^+} \ [(1-\gamma \ \cos\beta)(2G_{\beta}^{\dagger}G_{\beta} \ - \ 1) \ +1]\}P_+$$

$$+ \ \{- \ \frac{1}{2} \ \sum_{\alpha\epsilon S^-} \ [\ (1 \ - \ \gamma\cos\alpha) \ (2G_{\alpha}^{\dagger}G_{\alpha} \ - \ 1) \ +1]\}P_- \tag{6.71}$$

$$T(V) \ |\Phi_+> \ = \ 0 \qquad\qquad (6.72)$$

In addition we also have

$$T(V) \ |\Phi_-> \ = \ 0 \qquad\qquad (6.73)$$

but as $|\Phi_-> $ is not an allowed eigenstate it must be rejected. Equation (6.15) then suggests that $|\phi_e>$ the equilibrium state is related to $|\Phi_+>$, and is unique. This is to be expected as the one dimensional Ising model does not show a phase transition. Under the same set of transformations (6.40) the Ising Hamiltonian can be written

$$H \ = \ H^+ P_+ \ + \ H^- P_- \qquad\qquad (6.74)$$

where

$$H^\pm \ = \ -J \ \sum_{j=1}^{N} \ (f_j^\dagger - f_j)(f_{j+1}^\dagger + f_{j+1}) \qquad\qquad (6.75)$$

and $\pm$ refers to the anticyclic/cyclic boundary conditions (6.45). Bearing in mind (6.15) and (6.19) we may identify the states $|\Phi_\pm>$ as

$$|\Phi_\pm> \ = \ e^{-\beta/2 H^\pm} \ |0> \qquad\qquad (6.76)$$

Evidently the equilibrium state is given by

$$|\phi_e> \ = \ e^{-\beta/2 H^+} \ |\Phi_+> \qquad\qquad (6.77)$$

Using the fact that $H^\pm$ commutes, the states $|\Phi_\pm>$ may be related as

$$|\Phi_+> \ = \ e^{-\beta/2 (H^+ - H^-)} \ |\Phi_-> \qquad\qquad (6.78)$$

This relation will presently be used in evaluating the matrix elements which occur in the calculation of the time dependence of spin moments of the type $<\sigma_i^z \sigma_j^z \ \dots \ \sigma_p^z>_t$. The time dependence of spin operators diagonal in the σ_j^z representation is given by (6.12). Noting (6.43),

(6.13) and (6.76). It may be written as

$$\langle A^z \rangle_t = \langle \Phi_+ | \; A^z \; e^{tT(V)} \; | \phi_o \rangle \qquad (6.79)$$

Spectral decomposition, using the eigenstates of $T(V)$ yields

$$\langle A^z \rangle_t = \sum_j \langle \Phi_+ | \; A^z \; | \Phi_j \rangle \; e^{t\Lambda_j} \; \langle \Phi_j | \phi_o \rangle \qquad (6.80)$$

where the sum is over all j particle states $| \Phi_j \rangle$ as given in (6.69) and (6.70), and Λ_j the j particle eigenstates. The spin moments A^z may be classified into two types:

(a) A^z consists of an odd number of spin operators, and consequently an odd number of fermion operators, e.g. $\sigma_j{}^z$, $\sigma_j{}^z \sigma_1{}^z \sigma_p{}^z$, ...

(b) A^z consists of an even number of spin operators, and so an even number of fermion operators, e.g. $\sigma_j{}^z \sigma_1{}^z$, ...

To evaluate matrix elements $\langle \Phi_+ | A^z | \Phi_j \rangle$ we note that for odd operators as in case (a), the only non-vanishing matrix elements will be between the subspaces h_+ and h_-, whilst for 'even' operators as in case (b) the only contribution will be from matrix elements in h_+. We consider two examples to show how the matrix element may be evaluated in each case.

Case (a): $A^z = \sigma_1{}^z$.

We want to calculate matrix elements of the form

$$\langle \Phi_+ | \; \sigma_1{}^z G_\alpha^\dagger | \Phi_- \rangle; \quad \langle \Phi_+ | \; \sigma_1{}^z G_{\alpha_1}^\dagger G_{\alpha_2}^\dagger G_{\alpha_3}^\dagger \; | \Phi_- \rangle, \; \dots \qquad (6.81)$$

these being the allowed matrix elements between h_+ and h_-.

Proposition 6.1

(i) The value of $\langle \Phi_+ | \; \sigma_1{}^z G_\alpha^\dagger \; | \Phi_- \rangle$ is given by

$$\langle \Phi_+ | \; \sigma_1{}^z G_\alpha^\dagger | \Phi_- \rangle = \frac{e^{i\alpha} \; e^{i\omega(\alpha)}}{N^{\frac{1}{2}}} \; \frac{1}{ChV - e^{i\alpha}ShV} \qquad (6.82)$$

(ii) All other matrix elements of the type (6.81) vanish.

Proof: (i) Equation (6.78) relates the states $|\Phi_+\rangle$ and $|\Phi_-\rangle$. We may then write

$$\langle\Phi_+| \ \sigma_1{}^z G_\alpha^\dagger |\Phi_-\rangle \ = \ \langle\Phi_-| \ e^{-\beta/2(H^+-H^-)} \ \sigma_1{}^z G_\alpha^\dagger \ |\Phi_-\rangle \tag{6.83}$$

From (6.75) this may be written as

$$\langle\Phi_+| \ \sigma_1{}^z G_\alpha^\dagger |\Phi_-\rangle \ = \ ChV \ \langle\Phi_-| \ (f_1^\dagger + f_1) G_\alpha^\dagger |\Phi_-\rangle$$

$$- \ ShV \ \langle\Phi_-| \ (f_N^\dagger - f_N) G_\alpha^\dagger |\Phi_-\rangle \tag{6.84}$$

Using transformations (6.50) and (6.59) we obtain

$$\langle\Phi_+| \ \sigma_1{}^z G_\alpha^\dagger |\Phi_-\rangle \ = \ \frac{ChV}{N^{\frac{1}{2}}} \ e^{i\alpha} e^{i\omega(\alpha)} \{\Theta \ (e^{i\alpha}) + e^{i\alpha} \ thV\} \tag{6.85}$$

which is seen to be the same as (6.82) when (6.65) is used.

(ii) The fact that matrix elements involving three or more particles vanish is readily seen from (6.84), for these will involve unequal numbers of creation and annihilation operators.//

Proposition 6.1 has established that the only contributing matrix elements $\langle\Phi_+| \ \sigma_1{}^z |\Phi_j\rangle$ are from the one particle $G_\alpha^\dagger |\Phi_-\rangle$. It is not difficult to see that for n (odd) spin products only states containing $1 < n$ particles (1, odd) will make a non zero contribution.

The result of proposition (6.1) may be generalised by using the symmetry properties of the spin lattice Ω. To obtain $\langle\Phi_+| \ \sigma_j{}^z G_\alpha^\dagger |\Phi_-\rangle$ we observe that

$$\sigma_j{}^z \ = \ C^{-(j-1)} \ \sigma_1{}^z \ C^{(j-1)} \tag{6.86}$$

$$C|\Phi_+\rangle \ = \ |\Phi_+\rangle \tag{6.87}$$

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$$C \, G_\alpha^\dagger \, |\Phi_-\rangle = e^{i\alpha} \, G_\alpha^\dagger \, |\Phi_-\rangle \qquad (6.88)$$

where C is the translation operator through one lattice spacing, and generates the cyclic group C_N. Equations (6.86), (6.87) and (6.88) establish

$$\langle \Phi_+ | \, \sigma_j^z \, G_\alpha^\dagger \, |\Phi_-\rangle = e^{i(j-1)\alpha} \langle \Phi_+ | \, \sigma_1^z \, G_\alpha^\dagger |\Phi_-\rangle \qquad (6.89)$$

The time dependence of the transform

$$\sigma_\alpha^z = N^{-\frac{1}{2}} \sum_j e^{-ij\alpha} \, \sigma_j^z \qquad (6.90)$$

may be readily obtained by using (6.89), (6.82) and (6.80)

$$\langle \sigma_\alpha^z \rangle_t = e^{-t(1-\gamma\cos\alpha)} \cdot \langle \sigma_\alpha^z \rangle_0 \qquad (6.91)$$

which decays to its equilibrium value though only <u>one</u> relaxation time.

The case for even spin products is simpler, in that we have now to deal with matrix elements entirely within h_+. For example for the two spin moment $\langle \sigma_j^z \sigma_{j+1}^z \rangle_t$ we have:

<u>Proposition 6.2</u>

(i) States $|\Phi_j\rangle$ containing $1 > 2$ (1, even) particles make zero contribution to the time dependence.

(ii) The equilibrium state $\langle \sigma_j^z \sigma_{j+1}^z \rangle_{eq.}$ is given by

$$\langle \sigma_j^z \, \sigma_{j+1}^z \rangle_{eq.} = \langle \Phi_+ | \sigma_j^z \sigma_{j+1}^z | \Phi_+ \rangle \qquad (6.92)$$

(iii) $\qquad \langle \Phi_+ | \, \sigma_j^z \sigma_{j+1}^z G_{\beta_1}^\dagger G_{\beta_2}^\dagger | \Phi_+ \rangle =$

$$\frac{1}{N} \exp i \, (j\beta_1 + j\beta_2 + \omega(\beta_1) + \omega(\beta_2)) \cdot [\, e^{i\beta_2} \, \Theta \, (e^{i\beta_2}) - e^{i\beta_1} \, \Theta \, (e^{i\beta_1}) \,]$$

$$(6.93)$$

Proof: The proofs to these statements follow in a straightforward manner by using transformations (6.40), (6.50) and (6.60) and calculating the resulting expressions.//

Again a similar situation holds for the general case of a n (even) spin moment. The only contributing matrix elements involve states $|\Phi_j\rangle$ containing $1 \leq n$ (1 even) particles. The method of propositions (6.1) and (6.2) may be used to evaluate matrix elements of any spin moment, although naturally this becomes tedious for the higher order moments.

As an alternative method to the use of relation (6.78) in calculating matrix elements of odd spin moments, it is possible to apply a general method due to Abraham [34]. This method makes explicit use of the linear dependence relation (6.56) between the two classes of fermion operators F_β, and F_α to devise an integral equation for the appropriate matrix element. The method is applicable to a general class of functions $\Theta(z)$ to which (6.71) belongs. The results of proposition 6.1 may be reproduced in this way.

To summarise, we have made use of the various transformations needed to diagonalise the stochastic operator $T(V)$ to define new vacua $|\Phi_\pm\rangle$, and particle states $|\Phi_j\rangle$. This allowed us to use the free fermion character of the operator $T(V)$, and together with equation (6.78) provided a simpler alternative to the Felderhof method [29] in calculating matrix elements of spin moments occurring in (6.80). Moreover the properties of the fermion operators G_k, show clearly the relation between the order of the spin moment and the number of particle states contributing to its time evolution. The calculation is completed when the coefficient $\langle\Phi_j|\phi_o\rangle$ is evaluated for a particular choice of initial state $|\phi_o\rangle$.

Time delayed correlation functions of spin moments may be calculated by using equation (6.14), matrix elements occurring there being evaluated by the method of proposition 6.1 or 6.2. As an example we consider the one spin, time delayed correlation function $\langle\sigma_j^z(t)\sigma_k^z(o)\rangle$. From (6.14)

we find for this function

$$<\sigma_j{}^z(t)\ \sigma_k{}^z(o)> \ = \ <\Phi_+|e^{-tT(V)}\ \sigma_j{}^z\ e^{tT(V)}\sigma_k{}^z|\Phi_+> \qquad (6.94)$$

Spectral decomposition, use of proposition (6.1), equation (6.89) and considering the limit $N \to \infty$ for the infinite chain, we find

$$<\sigma_j{}^z(t)\ \sigma_k{}^z(o)> \ = \ \frac{1}{2\pi} \int_{-\pi}^{\pi} \frac{e^{-t(1-\gamma\cos\alpha)}\ e^{ir\alpha}}{\text{Ch}2V\ \cdot\ (1-\gamma\cos\alpha)}\,d\alpha \qquad (6.95)$$

where $r = |k-j|$.

The analytic properties of the integrand determine both the spatial and temporal development of the correlation function. We first note that at $t = 0$, the integral is readily evaluated to yield the equilibrium value [26]

$$<\sigma_j{}^z\sigma_k{}^z> \ = \ (\text{thV})^{|k-j|} \qquad (6.96)$$

To obtain the asymptotic form of (6.95) for large times t, and distances r, the integral is written as

$$<\sigma_j{}^z(t)\ \sigma_k{}^z(o)> \ = \ \frac{1}{2\pi} \int_C \frac{e^{-t(1-\gamma\cos\alpha)}\ e^{ir\alpha}}{\text{Ch}2V\ (1-\gamma\cos\alpha)}\,d\alpha \qquad (6.97)$$

where the contour C starts from $-\pi+i\infty$, passes through the saddle point $\alpha_o = i\text{Sh}^{-1}\frac{r}{\gamma t}$, to $\pi+i\infty$, (see figure 6.1)

The method of steepest descents then yields for the asymptotic form

$$<\sigma_j{}^z(t)\sigma_k{}^z(o)> \ \underset{\substack{t \to \infty \\ r \to \infty \\ r/\gamma t \ll 1}}{\sim} \ \frac{1}{\text{Ch}2V}\ \cdot\ \frac{1}{1-\gamma}\ \cdot\ \frac{e^{-t}\ e^{\gamma t\ -\ \frac{r^2}{2\gamma t}}}{\sqrt{2\pi\gamma t}} \qquad (6.98)$$
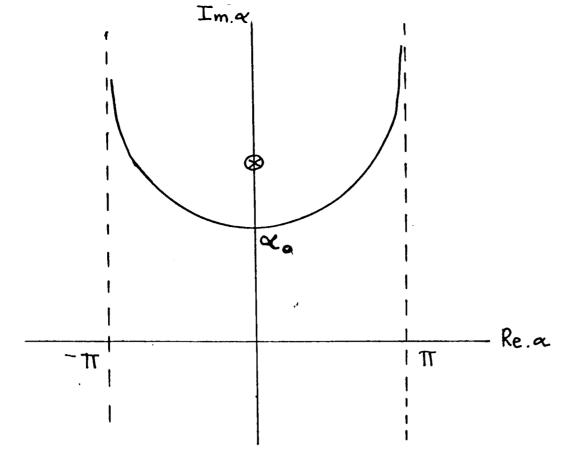
Figure 6.1. The contour C in the complex α plane

Equation (6.98) shows that in the regime $^r/\gamma t \ll 1$, and t, and r large, the behaviour of the correlation function resembles the solutions to the diffusion equation. The behaviour here is analogous to the Orstein Zernike approximation [35] in the equilibrium correlation functions.

Finally we note that the free energy per spin in the thermodynamic limit of the Ising chain.

$$-\beta f = \ln(2chV)$$

has a singularity at zero temperature (T = 0). If we take the view that this is a critical point, we may use the model to study irreversible behaviour, near this critical point. As $\gamma \to 1$, $T \to 0$ the basic relaxation rate of the α th mode becomes $\lambda_\alpha = 1 - \cos\alpha$. So for small momenta α (long wavelengths) the decay to equilibrium near the critical point becomes very slow.

APPENDICES AND REFERENCES

Appendix A

Both integrals may be readily evaluated by expressing them in terms of

$$U_p(\cos\phi) = \frac{1}{2\pi} P\!\!\int_0^{2\pi} \frac{\cos p\theta \ d\theta}{\cos\theta - \cos\psi} = \frac{\sin(p+1)\phi}{\sin\phi} \qquad (A.1)$$

This is a standard integral representation for Chebyshev polynomials of the second kind [24].

Appendix B

The integral along C^+ is

$$I = \frac{-1}{2\pi} \int_{-\pi}^{\pi} \frac{\sin(p+1)(a+i\alpha).\sin(x+i\alpha) \ dx}{\cos\theta - \cos(x+i\alpha)(e^{i2(N+1)(x+i\alpha)} - 1)} \qquad (B.1)$$

Substituting $z = e^{-\alpha}e^{ix}$, and using the residue theorem we have

$$I = \frac{1}{4\pi i} \oint_{|z|=e^{-\alpha}} \frac{(z^{(p+1)} - z^{-(p+1)})(z-z^{-1})dz}{(z^2 - 2z\cos\theta + 1)(1 - z^{2(N+1)})} = \cos(p+1)\theta$$

$$(B.2)$$

Appendix C

Proof of proposition 4.4

We want to calculate

$$\langle f_{nm}^{\dagger} f_{nm} \rangle_{\beta_L} = \frac{1}{M} \sum_1 \sum_j T_{nj}^2 \frac{1}{(e^{\beta_2(\lambda + \cos\theta_1)} + 1)} \qquad (C.1)$$

in the limit (i) $M, N_b \to \infty$, (ii) $N_s \to \infty$.

Using (4.21) and (4.16), and replacing the sum over 1 by integration over θ when $M \to \infty$ we write (C.1) as

$$\langle f_{nm}^{\dagger} f_{nm} \rangle_{\beta_2} = \frac{1}{2\pi} \int_0^{2\pi} d\theta \frac{1}{\pi i} \oint_C \frac{|G_{N_s}(p,\lambda)|^2}{G_{N_s}(\lambda) P_{N_s,N_b}(\lambda)} \frac{d\lambda}{(e^{\beta_2(\cos\theta + \lambda)} + 1)}$$

$$- \text{Res} (G_{N_s}(\lambda) = 0) \tag{C.2}$$
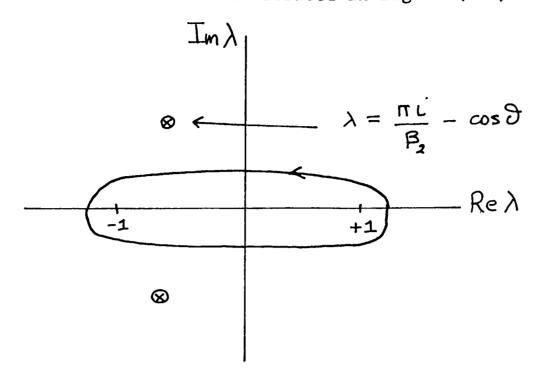
where C is the contour illustrated in figure (C.1)

Figure (C.1). Contour C enclosing the zeroes of $P_{N_s,N_b}(\lambda)$.

Using proposition (4.2) to take the limit $N_b \to \infty$ (C.2) can be written as

$$<f^\dagger_{nm} f_{nm}>_{\beta_2} = \frac{1}{2\pi} \int_0^{2\pi} d\theta \frac{\gamma^2}{\pi} \oint_C \frac{\sqrt{(1-\lambda^2)} |G_{N_s}(p,\lambda)|^2 \, d\lambda}{P_{N_s\infty}(\lambda) \, P_{N_s\infty}^*(\lambda)} \frac{1}{e^{\beta_2(\lambda+\cos\theta)}+1} \tag{C.3}$$

where C now encloses the cut from $[-1,1]$ in the λ plane, and $\gamma^2 \leq 1$. It is readily verified that (C.3) is equal to (4.51) from which the required result follows.

Appendix D

Wick-Bloch-de Dominicis Theorem:

Let Γ denote either of the fermion operators $\alpha^\dagger$, α where

$$[\alpha^\dagger_i, \alpha_j]_+ = \delta_{ij} \quad [\alpha^\dagger_i, \alpha^\dagger_j]_+ = 0 \tag{D.1}$$

and

$$[\Gamma_i, \Gamma_j]_+ = (i,j) \tag{D.2}$$

The pair (i,j) takes the values of the anticommutation rules defined in (D.1).

Consider $2n$ operators Γ_i $\{i = 1, \ldots 2n\}$ and let

$$<\Gamma_1 \ldots \Gamma_{2n}>_\beta \;=\; \frac{\text{Tr}(\Gamma_1 \ldots \Gamma_{2n} \; e^{-\beta H})}{\text{Tr} \; e^{-\beta H}} \qquad (D.3)$$

with

$$H \;=\; \sum_i \epsilon_i \alpha_i^\dagger \alpha_i$$

Theorem D.1

$$<\Gamma_1 \ldots \Gamma_{2n}>_\beta \;=\; \sum_p (-)^{\delta(p)} <\Gamma_{i_1} \Gamma_{i_2}>_\beta <\Gamma_{i_3} \Gamma_{i_4}>_\beta \ldots <\Gamma_{i_{2n-1}} \Gamma_{i_{2n}}>_\beta$$

$$(D.4)$$

where p is the permutation

$$p \;=\; \begin{pmatrix} 1 & 2 & \ldots & 2n \\ i_1 & i_2 & \ldots & i_{2n} \end{pmatrix} \qquad (D.5)$$

$\delta(p)$ the signature of the permutation, which is subject to the constraints

(i) $\qquad (i_1 < i_2); \quad (i_3 < i_4) \ldots (i_{2n-1} < i_{2n})$ $\qquad\qquad$ (D.6)

(ii) $\qquad\qquad i_1 < i_3 < i_5 < \ldots < i_{2n-1}$

Proof: Use (D.2) to systematically move Γ_1 to the extreme right.

$$<\Gamma_1 \ldots \Gamma_{2n}> \;=\; (1,2) <\Gamma_3 \Gamma_4 \ldots \Gamma_{2n}> - (1,3) <\Gamma_2 \Gamma_4 \ldots \Gamma_{2n}>$$

$$+ \ldots + (1,2n) <\Gamma_2 \ldots \Gamma_{2n-1}> - <\Gamma_2 \ldots \Gamma_{2n-1} \Gamma_{2n} \Gamma_1> \qquad (D.7)$$

We now use the identity

$$e^{\beta H} \alpha_i^\dagger e^{-\beta H} \;=\; e^{\beta \epsilon_i} \alpha_i^\dagger \qquad (D.8)$$

and trace invariance under cyclic permutations to show

$$\langle \Gamma_2 \Gamma_3 \cdots \Gamma_{2n} \Gamma_1 \rangle_\beta = e^{\pm \beta \epsilon_i} \langle \Gamma_1 \Gamma_2 \cdots \Gamma_{2n} \rangle \qquad (D.9)$$

Substituting into (D.7) and noting that

$$\frac{(i,j)}{1+e^{\pm \beta \epsilon_i}} = \langle \Gamma_i \Gamma_j \rangle_\beta \qquad (D.10)$$

we obtain

$$\langle \Gamma_1 \Gamma_2 \cdots \Gamma_{2n} \rangle = \langle \Gamma_1 \Gamma_2 \rangle \langle \Gamma_3 \cdots \Gamma_{2n} \rangle - \langle \Gamma_1 \Gamma_3 \rangle \langle \Gamma_2 \Gamma_4 \cdots \Gamma_{2n} \rangle$$

$$+ \ldots + \langle \Gamma_1 \Gamma_{2n} \rangle \langle \Gamma_2 \cdots \Gamma_{2n-1} \rangle \qquad (D.11)$$

This then provides a systematic way whereby (D.11) can be further

reduced to (D.4).

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