Chapter Seven

Quantum Monte Carlo Formalism for Spin Chains

7.1 Introduction: Quantum Effects in the Thermodynamics of Easy-Plane Ferromagnets

In Part I the classical dynamics of nonlinear excitations in 1-D easy-plane ferromagnets in the presence of an applied field in the easy plane has been studied. Although the dynamic kink properties were studied in detail, no thermodynamic quantities that can be measured experimentally were calculated, such as the specific heat, magnetic susceptibility or structure factor $\langle S^{\alpha}(0)\ S^{\beta}(x)\rangle$ measured in neutron scattering experiments. In this respect the analysis of Part 1 is incomplete, and it cannot in itself give detailed information about experiments. However, for Hamiltonian (2-1), there are other methods for obtaining the classical thermodynamics, especially by transfer integral methods (Loveluck et al. 1980, 1981, 1982, Leung and Bishop 1983, Kumar and Samalam 1982 and Pini and Rettori 1984), and classical soliton phenomenology (Currie et al. 1980, Mikeska 1978). In the latter, usually the Hamiltonian (2-1) is approximated by the sG Hamiltonian, and the classical phenomenology derives the thermodynamics from an ideal gas of sG solitons and spin waves, with breathers as a higher order effect. But in Part I we have conclusively demonstrated the limited validity of mapping (2-1) to the sG Hamiltonian. Therefore an ideal gas of sG excitations is inappropriate; the instability in the ferromagnetic kinks, causing the spins to tip out of the easy plane, is the reason. One would need to apply the phenomenology to an ideal gas of kinks, breathers and spin waves with properties as described in Chapters 2 and 3. Whether this can be done at present is unclear, especially considering the variety in the $K\bar{K}$ scattering phase diagram. One partial attempt along this line of thought is by Osano (1985), where

the branch II and branch III kinks are excluded from the calculation. Clearly, however, they will carry thermodynamic weight even at fields below b_c.

The transfer integral methods, however, should give the correct classical thermodynamics, since no particular assumptions about the kink dynamics are necessary. All the thermodynamic functions come from the largest eigenvalue of the transfer operator. Generally, however, experimental data (specific heat and magnetization) for the spin-1 $CsNiF_3$ (Ramirez and Wolf 1982, Rosinski and Elschner 1977) lie closer to the sG phenomenological theory (with a reduced soliton rest energy) than to the transfer integral theory using the full classical Hamiltonian (Loveluck et al. 1982, Pini and Rettori 1984). Somehow it appears that the out-of-plane motions are smaller than that given by the full classical Hamiltonian theory. Possibly this is a quantum effect which limits the out-of-plane motions, thereby making sG theory the more appropriate. This is certainly a likely possibility in such a low spin system. Note that these comments are even more appropriate for spin-$\frac{1}{2}$ CHAB, where data has also been presented (Kopinga et al. 1984) indicative of classical sG solitons with a renormalized rest mass. So a question to pose is: How should quantum mechanics be applied to this model? A further question is: Is quantum mechanics necessary to explain the experimental data for $CsNiF_3$ and CHAB, or does a slightly different classical model apply?

In order to fit classical sG phenomenological theory approximately to the experimental data for both $CsNiF_3$ and CHAB, it is necessary to use a soliton rest energy reduced from the classical value $E_0 = 8(Jg\mu_B B_x S^3)^{1/2}$. The reduction is approximately 20% for $CsNiF_3$ and 20% for CHAB. Mikeska (1982) and Maki (1980) have explained this energy reduction by quantizing the sG theory, while Kumar and Samalam (1982)

claim that it is entirely a classical renormalization due to out-of-plane fluctuations. Naturally one should quantize the full Hamiltonian from the start, not just the sG limit. But this has not been possible so far. Hence the reason for quantizing sG theory -- it is analytically tractable. But if the classical mapping of the full Hamiltonian (2-1) to the sG Hamiltonian has only a very limited range of validity, then we expect that mapping the full quantum Hamiltonian to the quantum sG Hamiltonian would also have only a very limited range of validity (for example, in velocity, field and anisotropy parameter space). So it seems that another approach is needed.

Quantum statistical mechanics for other model spin systems has been studied recently using finite temperature quantum Monte Carlo methods (Handscomb 1962, 1964, Suzuki 1976, Suzuki et al. 1977, Lyklema 1983, Cullen and Landau 1983 and DeRaedt et al. 1982). We have used these methods for this easy-plane ferromagnet. Cullen and Landau (1983) have studied the isotropic spin-$\frac{1}{2}$ Heisenberg chain and the analytically soluble xy model using what has been called the "checkerboard" decomposition of H. Here, their method (which is based on the work of Barma and Shastry 1978) is modified slightly and applied to the easy-plane (Heisenberg) ferromagnet with applied field in the easy plane, for both spin-$\frac{1}{2}$ and spin-1. We do not expect to make any definite statements about the possibility of quantum solitons in this system, but rather can only derive the thermodynamic functions such as the internal energy, specific heat, magnetization and susceptibility, without making any classical approximations (certainly the mapping of the full Hamiltonian (2-1) to the sG Hamiltonian was a classical operation). A further intention of the calculation will be to test the validity of the presumed Hamiltonian for explaining the experimental situation in $CsNiF_3$ and in CHAB.

In this chapter the general quantum Monte Carlo method used by Cullen and Landau (1983) will be reviewed, discussed in the context of an arbitrary 1-D spin Hamiltonian, for arbitrary spin S. Generally, Suzuki (1976, 1977) has shown a 1-D quantum statistical mechanics problem is equivalent to a 2-D classical statistical mechanics problem, through use of the general Trotter Formula (Trotter 1959). The energy of the effective 2-D lattice is given as a sum of "vertex" energies. The term vertex is taken from Baxter (1972), who solved for the partition function of the 1-D anisotropic Heisenberg model in the absence of a field. These vertex energies are related to matrix elements of spin operators of the original Hamiltonian. All thermodynamic quantities are obtained via expectation values of approprite variables (derivatives of the vertex weights) defined on the 2-D lattice. The expectation values will be found numerically using the standard (classical mechanics!) Metropolis et al. (1953) Monte Carlo algorithm. In Chapters 8 and 9 the method is applied specifically to the spin-$\frac{1}{2}$ material CHAB and the spin-1 material $CsNiF_3$, with the results compared to renormalized rest energy sG theory and available experimental data.

7.2 The 2-D Effective Classical Lattice: The Checkerboard Decomposition

First a review of the Suzuki-Trotter formalism will be given. This transformation essentially converts the trace operation for finding a partition function into a discrete path integral (or sum, in spin systems). The discussion is in the context of quantum Hamiltonian on 1-D lattices where the states are described by a set of discrete quantum eigenvalues (e.g. eigenvalues of $\hat{S}_n^z$ operators, or perhaps occupation numbers for fermion systems). We wish to find the partition function Z for a system of N particles,

$$Z = \mathrm{tr}\{\exp(-\beta\hat{H})\} = \sum_{\sigma} \langle\sigma|\exp(-\beta\hat{H})|\sigma\rangle \quad , \tag{7-1}$$

where the sum is over a complete set of states, each denoted by σ,

$$\sigma = \{S_1, S_2, S_3, \ldots S_N\} \quad . \tag{7-2}$$

Note that carets (e.g. $\hat{H}$) will be used to indicate operators, and β is the reciprocal temperature ($\beta = 1/k_B T$). The variables S_n are eigenvalues of an appropriately chosen operator, usually taken as $\hat{S}^z_n$. For a spin-S problem, since there are $2S + 1$ states per lattice site, the set of states contains $(2S + 1)^N$ members. Since it is generally difficult to perform this trace sum, or even evaluate the matrix elements, we resort to an approximate method which is more tractable.

The Trotter formula (Trotter 1959) is used to approximate the operator $\exp(-\beta\hat{H})$ by one for which the matrix elements are easier. The generalized Trotter formula for the exponential of a sum of k operators is

$$\exp\left(\sum_{i=1}^{k} \hat{\theta}_i\right) = \lim_{m\to\infty} \left[\prod_{i=1}^{k} \exp(\hat{\theta}_i/m)\right]^m \quad . \tag{7-3}$$

Here m is an integer called the Trotter index. Generally we will be concerned with Hamiltonians $\hat{H}$ which are the sum of two-body operators $\hat{H}_{n,n+1}$, which makes the choice of k = 2 convenient (or multiples of 2). Then usually each two-body Hamiltonian can be written as the sum of two parts, one which may be easily diagonalized, and denoted $\hat{H}^o_{n,n+1}$,

$$\hat{H} = \sum_{n} \hat{H}_{n,n+1} \tag{7-4a}$$

$$\hat{H}_{n,n+1} = \hat{H}^o_{n,n+1} + \hat{V}_{n,n+1} \quad . \tag{7-4b}$$

Since all the two-body Hamiltonians at even lattice sites commute with each other, and similarly for the odd sites, define

$$\hat{H}^{\circ}_{odd} = \sum_{n\ odd} \hat{H}^{\circ}_{n,n+1} \quad , \quad \hat{V}_{odd} = \sum_{n\ odd} \hat{V}_{n,n+1} \quad , \tag{7-5a}$$

$$\hat{H}^{\circ}_{even} = \sum_{n\ even} \hat{H}^{\circ}_{n,n+1} \quad , \quad \hat{V}_{even} = \sum_{n\ even} \hat{V}_{n,n+1} \quad , \tag{9-5b}$$

so that

$$\hat{H} = \hat{H}^{\circ}_{odd} + \hat{V}_{odd} + \hat{H}^{\circ}_{even} + \hat{V}_{even} \quad . \tag{7-5c}$$

$\hat{H}$ has now been written as a sum of 4 parts, so we apply the Trotter formula for k = 4 to obtain the mth order Trotter approximation to the partition function

$$Z^{(m)} = tr\ \left(e^{-\frac{\beta}{m}\hat{H}^{\circ}_{odd}}\ e^{-\frac{\beta}{m}\hat{V}_{odd}}\ e^{-\frac{\beta}{m}\hat{H}^{\circ}_{even}}\ e^{-\frac{\beta}{m}\hat{V}_{even}} \right)^{m} \quad . \tag{7-6}$$

But since all four operators $\hat{H}^{\circ}_{odd}$, $\hat{V}_{odd}$, $\hat{H}^{\circ}_{even}$ and $\hat{V}_{even}$ are sums of commuting operators, this can be rewritten as

$$Z^{(m)} = tr\{(\hat{L}_{odd}\ \hat{L}_{even})^{m}\} \tag{7-7a}$$

where

$$\hat{L}_{odd} = \prod_{n\ odd} \left(e^{-\frac{\beta}{m}\hat{H}^{\circ}_{n,n+1}}\ e^{-\frac{\beta}{m}\hat{V}_{n,n+1}} \right) \tag{7-7b}$$

$$\hat{L}_{even} = \prod_{n\ even} \left(e^{-\frac{\beta}{m}\hat{H}^{\circ}_{n,n+1}}\ e^{-\frac{\beta}{m}\hat{H}^{\circ}_{n,n+1}} \right) \quad . \tag{7-7c}$$

Introducing 2m - 1 additional complete sets of states, labeled by index r,

$$\sigma_r = \{S_{1,r}, S_{2,r}, S_{3,r}, \cdots S_{N,r}\} \quad , \tag{7-8}$$

we have

$$Z^{(m)} = \sum_{\sigma_1} \sum_{\sigma_2} \sum_{\sigma_3} \cdots \sum_{\sigma_{2m}} <\sigma_1|\hat{L}_{odd}|\sigma_2><\sigma_2|\hat{L}_{even}|\sigma_3)\ldots.<\sigma_{2m}|\hat{L}_{even}|\sigma_1> \quad . \tag{7-9}$$

Now it is easy to see that we have an expression for a <u>classical</u> partition function for a 2-D system of size N x 2m,

$$Z^{(m)} = \sum_{\sigma_1} \sum_{\sigma_2} \sum_{\sigma_3} \cdots \sum_{\sigma_{2m}} \prod_{<n,r>} e^{-\beta E_{n,r}} \quad . \tag{7-10}$$

Here the bracket notation <n,r> indicates a product restricted to terms in which n and r are both odd or both even, and the 2-D energy function $E_{n,r}$ for a block of four sites in the 2-D lattice, is given by the fundamental matrix element

$$e^{-\beta E_{n,r}} \equiv <S_{n,r}S_{n+1,r}|e^{-\frac{\beta}{m}\hat{H}^{o}_{n,n+1}} e^{-\frac{\beta}{m}\hat{V}_{n,n+1}}|S_{n,r+1}S_{n+1,r+1}> \quad . \tag{7-11}$$

The block of four sites in (7-11) is called a "vertex". Typically it represents a complicated four spin interaction dependent on temperature and the Trotter index m. The 2-D lattice consists of 2mN classical spin variables, which can have values from -S to +S in unit (or $\hbar$) increments. There are mN vertices in the 2-D lattice. Each classical spin variable belongs to two vertices. Since the only terms that contribute to the energy of the 2-D lattice are restricted to n and r both odd or both even, this has been refered to as a checkerboard decomposition of $\hat{H}$ (see Figure 7.1). In the limit $m \to \infty$, $Z^{(m)}$ becomes the exact partition function of the original quantum problem. For finite m, Suzuki (1984) has shown that the error in using a finite m approximation to Z varies as $1/m^2$.

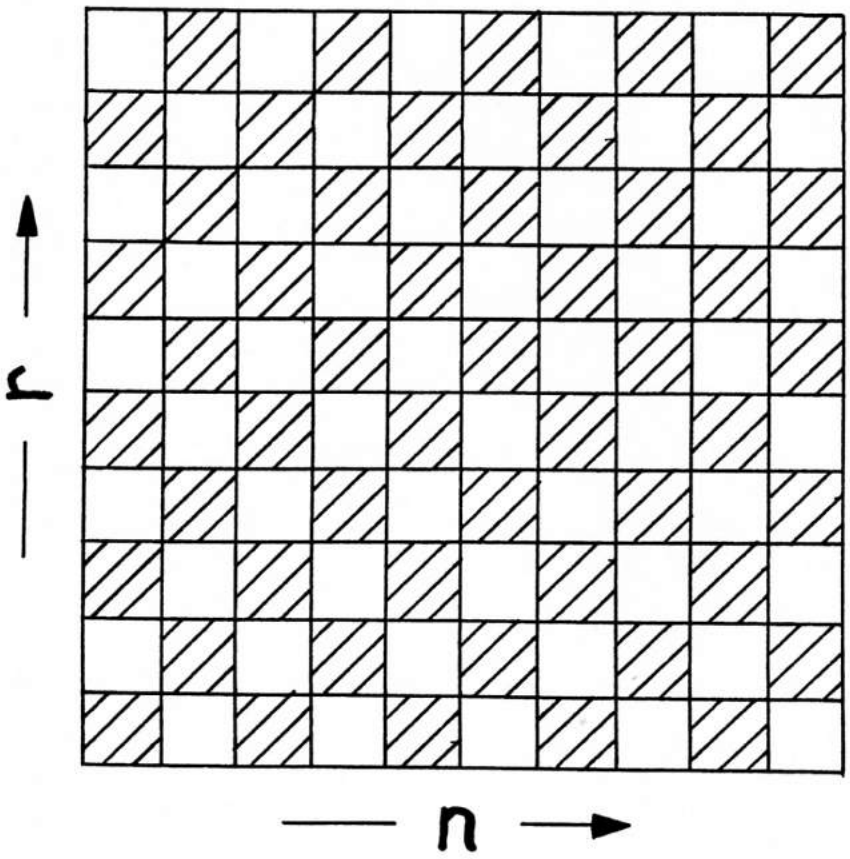

Figure 7.1 The checkerboard for N = 10, m = 5. A classical spin variable exists at each lattice site. Interactions occur only among spins which belong to the same shaded block, or "vertex".

This mapping is valid for any type of Hamiltonian, and in particular need not be restricted to spin problems. Also note that although it has been customary to assume that one uses eigenstates of $\hat{H}^{o}_{n,n+1}$ for the $S_{n,r}$ variables, this assumption is not necessary, and will not generally be taken here. Usually, however, it is used to simplify evaluation of the matrix elements.

A comment on the symmetry of the matrix elements in (7-11) is in order. Generally $\hat{H}^{o}_{n,n+1}$ and $\hat{V}_{n,n+1}$ do not commute, and so the order of the operators in (7-11) can introduce an asymmetry in these matrix elements with respect to the interchange of r and r + 1. Generally then we have formed a non-Hermitian operator. We are attempting to approximate matrix elements of $\hat{H}_{n,n+1}$, which certainly do have this Hermitian property, or time reversal symmetry (the r direction in the 2-D lattice is equivalent to a path integral direction in imaginary time). In order to restore this symmetry, we see that $\hat{H}_{n,n+1}$ could have been written as the sum of <u>three</u> parts: $\frac{1}{2}\hat{H}^{o}_{n,n+1}$, $\hat{V}_{n,n+1}$ and $\frac{1}{2}\hat{H}^{o}_{n,n+1}$. Then the vertex energy $E^{(m)}_{n,r}$ is given symmetrically by

$$e^{-\beta E_{n,r}} \equiv \langle S_{n,r}\ S_{n+1,r}| e^{-\frac{\beta}{2m}\hat{H}^{o}_{n,n+1}}\ e^{-\frac{\beta}{m}\hat{V}_{n,n+1}}\ e^{-\frac{\beta}{2m}\hat{H}^{o}_{n,n+1}} |S_{n,r+1}\ S_{n+1,r+1}\rangle \ . \tag{7-12}$$

This definition will be used for the vertex energies. Note that one can also define $E_{n,r}$ be interchanging $\hat{H}^{o}_{n,n+1}$ and $\hat{V}_{n,n+1}$ in (7-12).

The original 1-D lattice of quantum spins has been mapped approximately to a 2-D lattice of classical spins, with 2m rows, each having N classical spins. The lattice has periodic boundary conditions in the

Trotter direction because of the trace operation, and we will arbitrarily impose periodic boundary conditions in the spatial direction. We determine expectation values of quantum operators in the original problem as classical averages on the 2-D lattice, using classical 2-D Monte Carlo methods. Thermodynamic properties of the quantum system, such as the internal energy and specific heat, are found from appropriate derivatives of the partition function $Z^{(m)}$ with respect to temperature. These also become classical averages on the 2-D lattice. These averages, however, are of certain appropriate classical variables, derived in the next section (from Cullen and Landau 1983 and Barma and Shastry 1978).

7.3 Thermodynamics for the Quantum System

If the total energy of all the vertices of the 2-D lattice is denoted E_k, where the index k labels the state of the system, one can write the partition function

$$Z = \sum_k e^{-\beta E_k} \tag{7-13a}$$

with

$$E_k = \sum_{<n,r>} E_{n,r} \quad . \tag{7-13b}$$

The sum for Z is over all possible states of the 2-D lattice. Remembering that the vertex energies are functions of temperature, and so is E_k, then the internal energy $U^{(m)}$ is

$$U^{(m)} = -\frac{\partial}{\partial\beta} \ell n Z^{(m)} = (Z^{(m)})^{-1} \sum_k (E_k + \beta \frac{\partial E_k}{\partial \beta}) e^{-\beta E_k} \quad . \tag{7-14}$$

The internal energy is therefore not just the expectation value of the sum of the vertex energies, but includes another part. We can write this as

$$U^{(m)} = \langle F_k \rangle \quad \text{where} \quad F_k \equiv \frac{\partial}{\partial\beta}(\beta E_k) \quad . \tag{7-15}$$

Note that F_k is not the free energy. For an individual vertex one can define $f_{n,r}$, where

$$f_{n,r} \equiv \frac{\partial}{\partial\beta}(\beta E_{n,r}) \quad , \quad F_k = \sum_{\langle n,r \rangle} f_{n,r} \quad . \tag{7-16}$$

Similarly, the specific heat is given by a modified expectation value of the fluctuations in the total vertex energy

$$C^{(m)} = -\beta^2 \frac{\partial U^{(m)}}{\partial\beta} = \beta^2 \langle F_k^2 - G_k - \langle F_k \rangle^2 \rangle \tag{7-17a}$$

where

$$G_k = \frac{\partial F_k}{\partial\beta} = \sum_{\langle n,r \rangle} \frac{\partial}{\partial\beta} f_{n,r} = \sum_{\langle n,r \rangle} g_{n,r} \quad . \tag{7-17b}$$

And similarily, the magnetization and susceptibility are given by

$$M_i = \langle - \frac{\partial E_k}{\partial H_i} \rangle \tag{7-18a}$$

$$\chi_{ij} = \beta[\langle \frac{\partial E_k}{\partial H_i} \frac{\partial E_k}{\partial H_j} \rangle - M_i M_j] - \langle \frac{\partial^2 E_k}{\partial H_i \partial H_j} \rangle \quad . \tag{7-18b}$$

$\vec{H}$ is the applied field, i and j label components.

The classical Monte Carlo method is sketched out briefly. One starts with the 2-D system in some initial state, specified by the spin eigenvalues (of $\hat{S}_n^z$) of all the sites in the 2-D lattice. Then one attempts to make some small change in this initial configuration, by "flipping spins" (the classical ones) in units of . The change in energy ΔE that results from this more is computed. If $\Delta E < 0$, the move is accepted, and the process is repeated. If $\Delta E > 0$, then the move is accepted only with a probability $e^{-\beta\Delta E}$, and again the process is repeated. This algorithm generates a Markov chain whose limiting distribution is the Boltzman distribution. After some initial steps of the algorithm in order to allow transients to pass, one averages F_k, F_k^2, G_k and so on within the sequence of states generated by the algorithm, and the averages so obtained will be equivalent to expectation values over a Boltzman distribution.

The "dynamics" within the Monte Carlo algorithm is governed by the vertex energies $E_{n,r}$, or their weights $w_{n,r} = e^{-\beta E_{n,r}}$. In Chapters 7 and 8 vertex weights are computer for various spin-$\frac{1}{2}$ and spin-1 Hamiltonians. Spin flipping algorithms are presented, and results from simulations for CHAB and $CsNiF_3$ will be compared with experimental data (specific heat, susceptibility) and with the renormalized mass sG ideal gas theory.