Lattice diffusion and the Heisenberg ferromagnet

S. Alexander* and T. Holstein

Department of Physics, University of California, Los Angeles, California 90024

(Received 18 November 1977; revised manuscript received 22 February 1978)

It is shown that the master equation for a general diffusion problem with exclusion and symmetric binary transfer rates can be mapped exactly on the Schrödinger equation for an equivalent Heisenberg ferromagnet. Quantities of physical interest, e.g., the site occupation probability, are related to the lowest eignstates of the ferromagnet which play no thermodynamic role. The thermodynamics is only reflected in unobservable quantities such as the joint occupation probability of all sites. An additional result, obtained by elementary considerations, is the exact equation for the time evolution of the site-occupation probabilities. For symmetric transfer rates the equation reduces to a linear form in which exclusion effects are no longer present.

Huber, Hamilton, and Barnett[1] have recently pointed out the formal analogy between the rate equations in a diffusion problem and the linearized equations for spin deviations in a Heisenberg ferromagnet. Earlier, Kirkpatrick[2] had already related the resistor network problem to the spin stiffness of such a ferromagnet. The purpose of this note is to give these relationships a more precise meaning. We consider a general site-diffusion problem, with symmetric two-site transfer rates and exclusion of double occupancy of any site. We shall show that such a problem can be mapped exactly on an equivalent ferromagnetic Heisenberg problem. The quantities of physical interest are, however, quite different in the two cases. As a result, the diffusion problem is related to the ground-state properties of the ferromagnet and does not, in practice, reflect its thermodynamic behavior.

In general the site-occupation probabilities $\langle n_i \rangle$ obey the standard equation

$$\frac{d\langle n_i\rangle}{dt} = -\sum_j \left[W_{i\to j}\langle n_i(1-n_j)\rangle - W_{j\to i}\langle (1-n_i)n_j\rangle \right], \tag{1}$$

where for the occupation numbers one has $n_i = 0, 1$ and, as usual, the on square brackets denote statistical averages over the configurations of the system. We note that the occupation probabilities ($\langle n_i \rangle$) are continuous variables, The multiple site joint occupation probabilities (e.g., $\langle n_i n_j \rangle$) obey analogous equations. Thus, in general, Eq. (1) implies a hierarchy of equations for the joint occupation probabilities of successively larger numbers of sites. The derivation of Eq. (1) is standard and follows directly from the definition of the statistical averages on the lattice.

When the transfer rates are symmetric, the interference terms in Eq. (1) cancel

$$\frac{d\langle n_i\rangle}{dt} = -\sum_j W_{ij}(\langle n_i\rangle - \langle n_j\rangle) \tag{2}$$

and the equations no longer depend on the occupation density.

In principle, Eq. (1) should be derived from a master equation for the probability distribution for states of the whole system. To show the connection with the Heisenberg problem we do this explicitly. Consider first a two-site problem. The system has four possible states. We introduce a spin notation with spin up ($\sigma_i = +\frac{1}{2}$) describing occupied sites. The joint occupation probability of the two sites $\underline{\Pi}_{ij}(t)$ can then be regarded as a vector in the 4-dimensional space of product states $|\sigma_i \sigma_j\rangle$. It obeys the equation

$$\frac{d\underline{\Pi}_{ij}(t)}{dt} = 2W_{ij}(\underline{S}_i \underline{S}_j - \tfrac{1}{4})\underline{\Pi}_{ij}(t), \tag{3}$$

where the $\underline{S}_i$ are spin-$\frac{1}{2}$ vector operators. This is an operator form for the master equation of the two-site problem. Since the transfers are binary, the master equation for a large (N site) system becomes

$$\frac{d\underline{\Pi}(t)}{dt} = \sum_{i\neq j} W_{ij}(\underline{S}_i \underline{S}_j - \tfrac{1}{4})\underline{\Pi}(t), \tag{4}$$

where $\underline{\Pi}(t)$ is now a 2^N-dimensional vector describing the probability distribution of the states of the whole system.

Thus, the master equation for the diffusing system is identical to the Schrödinger equation for an equivalent Heisenberg system ($2W_{ij} \to J_{ij}$) for imaginary times and can be described in terms of the eigenfunctions and eigenvalues of that problem.

An interesting result is that the configuration of the diffusing system as a whole shows a thermodynamic behavior, with time playing the role of an inverse temperature. One has from Eq. (4),

$$\underline{\Pi}(t) = e^{-Ht}\underline{\Pi}(0), \tag{5}$$

where H is the Heisenberg Hamiltonian implied in Eq. (4). The probability of finding the system, at time t, in its initial state is

$$I_n(t)=\sum_{\cdots\sigma_i\cdots}\langle\cdots\sigma_i\cdots|e^{-Ht}|\cdots\sigma_i\cdots\rangle\underline{\Pi}_0^n(\cdots\sigma_i\cdots)\,, \tag{6}$$

where n is the number of occupied sites. If the initial configurations are uniform $[\underline{\Pi}_0^n(\cdots\sigma_i\cdots)=\text{const}]$, this leads to a relation with the free energy of the Heisenberg system at constant magnetization

$$\ln I_n(t)=-tF_{(N-2n)/2}(k_B/t)\,, \tag{7}$$

where $F_M(T)$ is the free energy of the Heisenberg system with total magnetization M at temperature T. Thus, $I_n(t)$ should exhibit a phase transition. This singularity is, however, of no physical interest because F is always of order N so that the transition occurs on a time scale

$$t\approx(WN)^{-1}\,. \tag{8}$$

We now want to show that quantities involving a small number of sites are related to the lowest eigenstates of the Heisenberg problem which play no thermodynamic role. We discuss explicitly only the site occupation probability. In the spin notation we have introduced, we can write the statistical average as

$$\langle n_i\rangle=\sum_{\{\sigma\}}n_i(\{\sigma\})\underline{\Pi}(t,\{\sigma\})=\langle\Phi|n_i|\Pi(t)\rangle\,, \tag{9}$$

where $\underline{\Phi}$ is a 2^N-dimensional vector all of whose elements are unity (1) and

$$n_i=S_z^i+\tfrac{1}{2}\,. \tag{10}$$

Finally,

$$\frac{d\langle n_i\rangle}{dt}=\langle\Phi|n_i\sum_{j,k}W_{jk}(\underline{S}_j\underline{S}_k-\tfrac{1}{4})|\Pi(t)\rangle\,. \tag{11}$$

This must be equivalent to the linear equation for the $\langle n_i\rangle$ [Eq. (2)].

To see how this comes about, we notice that Φ is an eigenvector of the "Heisenberg Hamiltonian" with the maximum spin ($S_{\max}=\frac{1}{2}N$) and eigenvalue zero. The single spin operator n_i operating to the left can only connect this state to eigenfunctions with total spin $S_{\max}$ and $(S_{\max}-1)$. These are the Bloch single spin-wave states.[3] They are described by the linear equations. An explicit calculation would of course lead to Eq. (2).

More generally we see that a ν site joint occupation probably would only involve states with

$$S_{\max}-\nu\leq S\leq S_{\max}\,.$$

In other words, only states with, at most, ν spin waves are involved. Such eigenstates (for microscopic ν) play no role in the thermodynamic behavior.

The relationship derived is of interest mainly in relating the nontrivial solutions of the two problems for random systems.[1,4,5] We also note that there seems to be some confusion in the recent literature as to the proper form of the rate equations, their derivation and range of validity. The procedure we outline may therefore also serve as an explicit proof of the validity of Eqs. (1) and (2) if such a proof is indeed required.

ACKNOWLEDGMENTS

We would like to thank Professor R. Orbach for very helpful discussions. Supported in part by the NSF Grant No. DMR75-19544 and by the Office of Naval Research ONR N00014-75-C-0245 P3.

*Permanent address: The Racah Institute of Physics, the Hebrew University, Jerusalem, Israel.

[1] D. L. Huber, D. S. Hamilton, and B. Barnett, Phys. Rev. B 16, 4642 (1977).

[2] S. Kirkpatrick, Solid State Commun. 12, 1279 (1973).

[3] F. Bloch, Z. Phys. 61, 206 (1930).

[4] H. E. Stanley, R. J. Birgeneau, P. J. Reynolds, and J. F. Nicoll, J. Phys. C. 9, 1533 (1976).

[5] T. Holstein, S. K. Lyo, and R. Orbach, Phys. Rev. Lett. 36, 891 (1976).