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Relaxation Phenomena in an Ising Spin System*

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The kinetics of an Ising model is formulated by the method of thermodynamics of irreversible processes. From the expression for the entropy production generalized forces and fluxes are determined. By introducing kinetic coefficients which satisfy the Onsager relation, the kinetic equations are obtained. By solving these equations a set of relaxation times is obtained. In terms of these relaxation times two initial value problems are solved.

For consideration we take a set of N identical Ising spins of magnitude 1/2. In thermodynamic equilibrium these spins behave similarly, and one can discuss the long range or the short range order. In a time dependent phenomenon, this is not the case and all spins behave differently at a given instant of time. There is a certain phase relation between motions of neighboring spins.

We assume the following form for the total distribution function:

$$f_N = \Pi f_n(\sigma_n) ,$$
$$\sigma_n = \pm 1 ,$$
$$\sum_{\sigma_n} f_n(\sigma_n) = 1 .$$

This form corresponds to Bragg-Williams approximation in thermal equilibrium condition, but here we discuss fluctuations in the neighborhood of the equilibrium condition.

The energy and the entropy of the system are given by

$$U_N = -[J(a)/2] \sum_{\langle m,n \rangle} \sum_{\sigma_m} \sum_{\sigma_n} \sigma_m \sigma_n f_n(\sigma_n) f_m(\sigma_m) + U_{NO}(a) ,$$

$$S_N = -k \sum_{\sigma_n} \sum_{n} f_n(\sigma_n) \ln f_n(\sigma_n) ,$$

where $J(a)$ is the exchange integral between two neighboring spins as a function of lattice constant a, and $U_{NO}(a)$ is the lattice energy other than the exchange interaction again as a function of lattice constant.

Deviation of the Helmholtz free energy from an equilibrium value is given by

$$\Delta F_N = \frac{1}{2}\left\{\left(\frac{\partial^2 U_{NO}}{\partial a^2}\right) - \left(\frac{\partial^2 J}{\partial a^2}\right)\left(\frac{zN\sigma_0^2}{2}\right)\right\}(a-a_0)^2 - \left(\frac{\partial J}{\partial a}\right) \sum_{\langle m,n \rangle} \sum_{\sigma_m} \sum_{\sigma_n} f_m^{(0)} \{f_n - f_n^{(0)}\}(a-a_0)$$

$$-2^{-1} J(a_0) \sum_{\langle m,n \rangle} \sum_{\sigma_m} \sum_{\sigma_n} \sigma_m \sigma_n \{f_m - f_m^{(0)}\}\{f_n - f_n^{(0)}\} + 2^{-1} kT \sum_{m} \sum_{\sigma_m} \{f_m^{(0)}\}^{-1} \{f_m - f_m^{(0)}\}^2 ,$$

where z is the number of nearest neighbors, σ_0 the equilibrium value of σ, a_0 the equilibrium lattice constant and $f_m^{(0)}$ is the equilibrium distribution function. Those equilibrium values are found by the minimum conditions for the free energy.

$$\sigma_0 = \tanh \beta , \qquad \beta = zJ(a_0)\sigma_0/kT, \qquad f_n^{(0)}(\sigma_n) = 2^{-1} \operatorname{sech} \beta \cdot \exp(\beta \sigma_n) .$$

By the usual argument we find

$$\sigma_0 = 0 , \qquad \text{when} \qquad kT/zJ(a_0) = 1 .$$

According to the theory of irreversible thermodynamics deviations of the distribution functions $f_m - f_m^{(0)}$ are regarded as the generalized fluxes. Then one can introduce corresponding generalized forces by the following equations

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$$X_m(\sigma_m)=\delta(\Delta F/T)/\delta(f_m-f_m^{(0)})$$
$$=(k/f_m^{(0)})(f_m-f_m^{(0)})-(J/2T)\sum_{\langle n\rangle}\sum_{\sigma_n}\sigma_m\sigma_n(f_n-f_n^{(0)})-T^{-1}(\partial J/\partial a)\sum_{\langle n\rangle}\sum_{\sigma_n}\sigma_m\sigma_n f_n^{(0)}(a-a_0)\,.$$

In terms of Onsager kinetic coefficients L_{mn}, one can set up kinetic equations in the following form:

$$\frac{df_m}{dt}=\sum_n\sum_{\sigma_n}L_{mn}(\sigma_m,\sigma_n)X_n(\sigma_n)\,.$$

In the following we assume a single spin-flip assumption. This leads to

$$L_{mm}(\sigma_m,\sigma_m')\neq 0\,,\qquad L_{mm}(\sigma_m,\sigma_m)\neq 0\,,\qquad L_{mn}(\sigma_m,\sigma_n)=0\,.$$

Introducing a new kinetic coefficient $w(\sigma_m,\sigma_m')$ by

$$L(\sigma_m,\sigma_m')=w(\sigma_m,\sigma_m')f_m^{(0)}(\sigma_m')\,,$$

the Onsager relation becomes

$$w(\sigma_m,\sigma_m')f_m^{(0)}(\sigma_m')=w(\sigma_m',\sigma_m)f_m^{(0)}(\sigma_m)\,.$$

By the normalization condition for the distribution function one obtains

$$w(++)+w(-+)=0\,,\qquad w(+-)+w(--)=0\,.$$

Combining these with the Onsager relations one gets

$$w(++)=-w(-+)=-\nu e^{-\beta}\,,\qquad w(--)=-w(+-)=-\nu e^{\beta}\,,$$

where ν is given by

$$w(+-)f^{(0)}(-)=w(-+)f^{(0)}(+)=2^{-1}\,\mathrm{sech}\beta\cdot\nu$$

Introducing an instantaneous average $\langle\sigma_n\rangle$ by

$$\langle\sigma_n\rangle=\sum\sigma_n f_n(\sigma_n)$$

one obtains the following kinetic equation

$$\frac{d\langle\sigma_m\rangle}{dt}=-2\nu k\cosh\beta\{\langle\sigma_m\rangle-\sigma_0\}+\left(\frac{\nu J}{T}\right)\cosh\beta(1-\sigma_0\tanh\beta)\sum_{\langle n\rangle}\{\langle\sigma_n\rangle-\sigma_0\}\,.$$

For a simple cubic lattice, we introduce

$$\langle\sigma_m\rangle-\sigma_0\ \rightarrow\ x_{l,m,n}$$
$$\alpha=2\nu k\cosh\beta\,,\qquad \gamma=(\nu J/T)\cosh\beta(1-\sigma_0^2)\,,$$

then the kinetic equation becomes

$$\frac{dx_{lmn}}{dt}=-\alpha x_{lmn}+\gamma\{x_{l+1,m,n}+x_{l-1,m,n}+x_{l,m+1,n}+x_{l,m-1,n}+x_{l,m,n+1}+x_{l,m,n-1}\}\,.$$

Assuming a periodic boundary condition one introduces a Fourier transform:

$$x_{lmn}=N^{-1/2}\sum_{\lambda}\sum_{\mu}\sum_{\nu}\alpha_{\lambda\mu\nu}\exp 2\pi i(l\lambda+m\mu+n\nu)/N^{1/3}\,,$$

then

$$\frac{da_{\lambda\mu\nu}}{dt}=-\alpha a_{\lambda\mu\nu}+2\gamma\left\{\cos\frac{2\pi\lambda}{N^{1/3}}+\cos\frac{2\pi\mu}{N^{1/3}}+\cos\frac{2\pi\nu}{N^{1/3}}\right\}\,.$$

Assuming

$$a_{\lambda\mu\nu}=a_{\lambda\mu\nu}(0)\exp(-t/\tau_{\lambda,\mu,\nu})$$

One obtains

$$(\tau_{\lambda\mu\nu})^{-1}=\alpha-2\gamma\left\{\cos\frac{2\pi\lambda}{N^{1/3}}+\cos\frac{2\pi\mu}{N^{1/3}}+\cos\frac{2\pi\nu}{N^{1/3}}\right\}.$$

For illustration we solve a relaxation equation for the linear chain with the initial condition

$$\langle\sigma_N(0)\rangle=\sigma_1\,,\qquad \langle\sigma_m(0)\rangle=\sigma_0\,,$$

then we obtain

$$\langle\sigma_m(t)\rangle-\sigma_0=N^{-1/2}(\sigma_1-\sigma_0)\sum_l\exp\left(-\frac{t}{\tau_l}+\frac{2\pi ilm}{N}\right).$$

In the limit $N\to\infty$ we can transform to a continuous variable

$$\langle\sigma_m(t)\rangle-\sigma_0=(\sigma_1-\sigma_0)e^{-\alpha t}I_m(\gamma t)\,,\ \langle\sigma_N(t)\rangle-\sigma_0=(\sigma_1-\sigma_0)e^{-\alpha t}I_0(\gamma t)\,,$$

where $I_m(\gamma t)$ is the Bessel function of imaginary argument. The spin at the N-th lattice point starts with the value σ_1 initially but approaches σ_0 with time exponentially. The spin at the m-th lattice point starts with the equilibrium value σ_0 initially but deviates from the equilibrium value monotonically until the deviation reaches a maximum then decreases and eventually approaches the equilibrium value back again.

It is straightforward to extend to a three-dimensional case and the result is

$$\langle\sigma_{lmn}(t)\rangle-\sigma_0=(\sigma_1-\sigma_0)e^{-\alpha t}I_l(\gamma t)I_m(\gamma t)I_n(\gamma t)\,.$$

The time development is quite similar to that of the one-dimensional lattice. The farther the location of the spin (l, m, n) from the origin, the slower the response to the excitation.

The above solution is essentially a Green's function of the problem, one can solve more general time dependent problems in terms of this Green's function.

DISCUSSION

R. KUBO: Why did you consider the change of the lattice constants? I suppose it has nothing to do with the essential points of the theory.

T. TANAKA: It is necessary to consider the variation in the lattice constant in order to calculate the sound wave attenuation coefficient, but that is not necessary for the discussion of the initial value problem.

R. KUBO: You assumed only the diagonal elements of the matrix of kinetic coefficients. May I ask what are the assumptions you made for deriving the difference equation of relaxation?

T. TANAKA: The reason why only the diagonal elements of the matrix of kinetic coefficients are retained is to make the dynamical problem as simple as possible. This approximation may be called a single spin-flip assumption. One can of course include more kinetic coefficients without much mathematical difficulty.