Transport Coefficients near the Critical Point: A Master-Equation Approach

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Kawasaki has shown how to construct a nonequilibrium theory which relaxes to an equilibrium described by the standard Ising model. The main significance of Kawasaki's work is his proof that transport coefficients do not diverge near the critical point in his model. In this paper, his approach is generalized. Two master-equation models of transport are examined: one gives spin diffusion and thermal diffusion but no sound waves; the other gives thermal diffusion and sound waves. The first model involves a Hermitian transition matrix in the master equation. The Hermiticity enables one to prove a variational theorem which requires the transport coefficients to be finite. However, sound waves appear as complex eigenvalues of the relaxation time. Hence, they must come from a non-Hermitian master equation. A model is constructed which includes sound waves. In this case, the proof of the finiteness of transport coefficients fails. Aside from formal questions, the main physical point of this paper is the speculation that infinities in transport coefficients might be tied to the existence of oscillatory transport modes (like sound waves) coupled into the dynamics of the phase transition.

I. INTRODUCTION

IN a very interesting series of papers,[1,2,3] Kawasaki has investigated the behavior of transport coefficients near the critical point. Basically, his model is an Ising model in which spins on neighboring sites are interchanged at a given rate. The details of the interchange are arranged so that the system relaxes to the usual Ising model equilibrium state. This model then describes spin diffusion in an insulator or particle diffusion in a binary alloy like β brass.

Kawasaki formulates his model in terms of a master equation. Glauber[4] and Heims[5] have also applied master equations to Ising models. However, a special feature of Kawasaki's work is a variational theorem which enables him to calculate an upper bound to the transport coefficients in his model. This upper bound is finite so that the exact transport coefficients derived from this model cannot possibly diverge near the critical point.

This model is a rough description of the situation in materials[6] such as β brass. Indeed, experiment indicates that the particle self-diffusion coefficient does not appear to diverge near the critical point in these materials.

However, other critical points are accompanied by divergent transport coefficients. In the liquid gas phase transition the thermal conductivity λ_T appears to diverge as the critical point is approached.[7,8] In iron,[9] the spin diffusivity does not appear to go very strongly to zero, so that the spin diffusion transport coefficient is probably diverging rather strongly. There are theoretical arguments[10–12] and experimental evidence[13] that the shear viscosity η diverges at the critical point of fluid mixtures. The thermal conductivity apparently diverges as the superfluid transition of He^4 is approached from above.[14,15]

Therefore, Kawasaki's arguments seem to work well for the specific situation in which the physics is closest to the conditions of his model. However, in other situations, Kawasaki's basic conclusion—that the transport coefficients are finite—fails.

At first sight this failure appears to be a great mystery. The arguments for finite transport coefficients seem very simple and general: The existence of a master equation, the proof of a variational theorem, and finally the explicit calculation of a finite upper limit. However, there turns out to be one feature of the argument which is not universally applicable. The proof of the variational theorem depends upon the Hermitian nature of

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the transition matrix in the master equation. The transition matrix then has real eigenstates and these eigenvalues have the physical significance of being the relaxation times of the different modes in the system. Of course, diffusion processes involve real relaxation times. For example, thermal diffusion produces an inverse relaxation time for a disturbance with wave vector q which is $\tau^{-1}=(\lambda_T/\rho C_p)q^2$. But, sound waves and spin waves are oscillatory phenomena. Insofar as they are not damped, they are represented by pure imaginary relaxation times. When damping is included, these eigenvalues of the transition matrix become complex. Hence, as soon as we admit sound waves, we must abandon the Hermitian transition matrix in the master equation. Then the proof of the finiteness of transport coefficients fails because the variational principle no longer exists. It seems possible, at least, that infinities in transport coefficients are tied to the existence of oscillatory modes coupled into the dynamics of the phase transition and their consequent non-Hermitian representation in the transition matrix.

In this paper, these basic ideas are examined through the consideration of master-equation models of transport phenomena. In the next section, the formalism of master equations is described with a view to seeing how equilibrium behavior and conservation laws are fixed into the structure of these equations. Section III describes a model for transport which relaxes to the standard Ising model in equilibrium. The spin-exchange processes are constructed in such a manner as to conserve the Ising model energy and the total spin. Therefore, the master equation implies two diffusive transport modes: spin diffusion and thermal diffusion. For $T>T_c$ and zero magnetic field, we prove that the two transport coefficients involved are finite at T_c. (As a consequence, the spin diffusivity goes to zero as the inverse susceptibility and the thermal diffusivity vanishes as the inverse specific heat).

Section IV describes a model of dynamical behavior that includes sound waves. This model is then appropriate for fluids. To bring in sound waves, a momentum variable is introduced in addition to the "spin" variable of the standard lattice gas.[14,15] The model is arranged so that, in equilibrium, the momentum may be eliminated from the partition function in a trivial way. This same elimination occurs in classical statistical mechanics. Then, the remaining partition function is chosen to represent the lattice gas or Ising model.

In this model, the momentum is tied into the dynamics in a nontrivial manner. Particles tend to move in the direction of their momentum. Coupled conservation laws for momentum, number, and energy are shown to reduce to standard linearized hydrodynamic equations. The model then includes both thermal diffusion and sound waves.

However, the transition matrix of this model is non-Hermitian. The proof that the transport coefficients are finite at the critical point fails. Therefore, the divergence or nondivergence of these transport coefficients in the fluids is left as an open question in this analysis.

II. MASTER EQUATIONS

In this section, we review some of the formalism of master equations and construct a notational system which will be useful for the rest of the paper.

A. Notation

We describe a system like the classical Ising model. There is a lattice and at each lattice site, $\mathbf{r}$, there is a spin variable $\sigma_\mathbf{r}$ which can take on two values, ± 1. The complete state of the system is given by specifying all the values of all these spin variables. We find it convenient to associate a state vector with every spin configuration. This state vector is written as $|\alpha\rangle$, where α is an index which defines all the values of all the different spins.

The time dependence of the model is given by specifying the equation of motion obeyed by $p_\alpha(t)$, the properly normalized probability of finding the system in the state α. We take this to be a first-order equation

$$\frac{d}{dt}p_\alpha(t)=\sum_\beta T_{\alpha\beta}p_\beta(t)\,, \tag{2.1}$$

so that a determination of all the $p_\alpha(t)$ at any time will define the values of the probabilities at all later times. If $\beta\neq\alpha$, $T_{\alpha\beta}$ is the probability per unit time that the system will hop from state β to state α while $-T_{\alpha\alpha}$ is the rate of hopping out of the state α.

It is convenient to write the purely classical master equation, Eq. (2.1), in a matrix form. To do this, let us assume that the basis states $|\alpha\rangle$ are orthonormal so that

$$\langle\alpha|\beta\rangle=\delta_{\alpha\beta}. \tag{2.2}$$

This equation means that two basic states $|\alpha\rangle$ and $|\beta\rangle$ are orthogonal if the value of the spin at any site is different in state $|\alpha\rangle$ from that in state $|\beta\rangle$. The statistical state of the system at time t is given by

$$|t\rangle=\sum_\alpha p_\alpha(t)|\alpha\rangle\,,$$

so that $\langle\alpha|t\rangle$ is the probability of finding the system in the state $|\alpha\rangle$. If we also define a transition matrix

$$\mathbf{T}=\sum_{\alpha\beta}|\alpha\rangle T_{\alpha\beta}\langle\beta|\,, \tag{2.3}$$

then Eq. (2.1) can be written in the simple form

$$(d/dt)|t\rangle=\mathbf{T}|t\rangle. \tag{2.4}$$

An important auxiliary quantity in the analysis is the special-state vector

$$|\,\rangle=\sum_\alpha|\alpha\rangle. \tag{2.5}$$

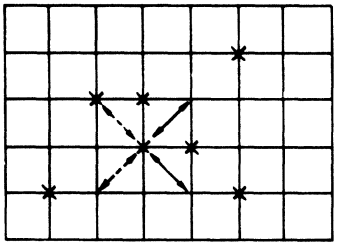


FIG. 1. Some interchanges described by the T^A matrix. The x's represent $\sigma_r=+1$ at the lattice site while the unmarked intersections represent $\sigma_r=-1$ at that site. The solid lines indicate allowed interchanges between spin "up" and spin "down". The broken lines indicate forbidden interchanges. The forbidden interchanges shown above involve either a change in energy or the interchange of two like spins. There are other allowed and nonallowed interchanges for the situation shown above which are not shown for the sake of clarity.

For example, we can use this quantity to give a compact formulation of the concept of conservation of probability. This is the statement

$$\frac{\partial}{\partial t}\langle\,|\mathbf{t}\rangle=\frac{\partial}{\partial t}\sum_\alpha p_\alpha(\mathbf{t})=\frac{\partial}{\partial t}1=0.$$

From Eq. (2.5) we then see that the statement of conservation of probability or detailed balance is

$$\langle\,|\mathbf{T}=0 \qquad \text{detailed balance.} \quad (2.6)$$

Given any physical quantity, X which has values X_α in the state α we define a diagonal operator representation of that quantity as

$$\mathbf{X}=\sum_\alpha |\alpha\rangle\langle\alpha|X_\alpha. \quad (2.7)$$

For example, the spin at site $\mathbf{r}$ is given by taking $X_\alpha=(\sigma_r)_\alpha$ to have the values ±1 depending upon the sign of σ_r in the state α. The statistical average of X at time t is given by

$$\langle X\rangle_t=\langle\,|\mathbf{X}|t\rangle. \quad (2.8)$$

From Eq. (2.5) this obeys the equation of matrix

$$(d/dt)\langle X\rangle_t=\langle\,|\mathbf{XT}|t\rangle, \quad (2.9)$$

when we apply the detailed balancing condition (2.6) we find that this equation of motion can also be written as

$$(d/dt)\langle X\rangle_t=\langle\,|[\mathbf{X},\mathbf{T}]|t\rangle. \quad (2.10)$$

Transport properties are intimately linked with conservation laws. We denote the n conserved quantities in the system by the symbols C_i, $i=1, 2, \cdots n$. For example, in the analysis of the usual Ising-model ferromagnet, we would like to have the total magnetization

$$\mathbf{M}=\sum_{\mathbf{r}}\sigma_r=\mathbf{C}_1, \quad (2.11a)$$

and the Hamiltonian

$$\mathbf{H}=-\sum_{\langle\mathbf{r},\mathbf{r}'\rangle}\sigma_r\sigma_{r'}=\mathbf{C}_2 \quad (2.11b)$$

be conserved. [In Eq. (2.11b), $\langle\mathbf{rr}'\rangle$ indicates that the sum is to be taken over all pairs of nearest neighbors.] From Eq. (2.10) we can see that the conservation laws

$$(d/dt)\langle C_i\rangle_t=0$$

can be equivalently stated as commutation relations

$$[\mathbf{C}_i,\mathbf{T}]=0 \qquad \text{conservation laws} \quad (2.12)$$

B. A Specific Example

It is easy to construct transition matrices, $T_{\alpha\beta}$, which satisfy the requirements stated above. For example, consider a model in which Ising spins are distributed upon a square or cubic lattice. Let there be a probability per unit time w^A that any pair of next-nearest-neighbor spins will interchange their values of σ_r. This interchange is only allowed if the process does not change the total energy H. Examples of possible and impossible interchanges are shown in Fig. 1.[16]

Mathematically, this model is represented by

$$\mathbf{T}=\mathbf{T}^A=\tfrac{1}{2}\sum_{r,r'}\mathbf{T}_{r,r'}{}^A, \quad (2.13)$$

with

$$\mathbf{T}_{r,r'}{}^A=w^A(\mathbf{I}_{r,r'}-1)\Delta_{r,r'}{}^A. \quad (2.14)$$

Here $\mathbf{T}_{r,r'}{}^A$ is the operator which describes the transition probability resulting from interchanges of spins at the nearest neighbor sites $\mathbf{r}$ and $\mathbf{r}'$. The off diagonal operator $\mathbf{I}_{r,r'}$ represents the actual interchange process

$$\mathbf{I}_{r,r'}\sigma_r=\sigma_{r'}\mathbf{I}_{r,r'},$$
$$\mathbf{I}_{r,r'}\sigma_{r'}=\sigma_r\mathbf{I}_{r,r'}.$$
$$[\mathbf{I}_{r,r'},\sigma_{r_1}]=0 \text{ for } \mathbf{r}_1 \text{ different from } \mathbf{r} \text{ and } \mathbf{r}'. \quad (2.15)$$

Of course, $\mathbf{I}_{r,r'}$ obeys

$$\mathbf{I}_{r,r'}=\mathbf{I}_{r',r},$$
$$(\mathbf{I}_{r,r'})^2=1. \quad (2.16)$$

Note that $\mathbf{I}_{r,r'}$ is not a matrix in $\mathbf{r}$ and $\mathbf{r}'$; instead these coordinates are labels for $\mathbf{I}_{r,r'}$. The matrix elements of $\mathbf{I}_{r,r'}$ are between states with specified values of the spin variables, i.e.,

$$\langle\bar\sigma_r\bar\sigma_{r'}|\,\mathbf{I}_{r,r'}\,|\sigma_r\sigma_{r'}\rangle=\delta(\bar\sigma_r,\sigma_{r'})\delta(\bar\sigma_{r'},\sigma_r).$$

The delta symbol, $\Delta_{r,r'}{}^A$, delimits the allowed interchanges. It is defined by

$$\Delta_{r,r'}{}^A=\begin{cases}1 \text{ if } \begin{cases}\mathbf{I}_{r,r'}\mathbf{H}\mathbf{I}_{r,r'}=\mathbf{H}\\ \sigma_r=-\sigma_{r'}\\ \mathbf{r} \text{ and } \mathbf{r}' \text{ are next-nearest neighbors}\end{cases}\\ 0 \text{ otherwise}\end{cases} \quad (2.17)$$

[16] This choice of the transition matrix makes the magnetization on two different sublattices separately conserved. However, we may add nearest neighbor or next-next-nearest neighbor interchanges to the transition matrix to destroy this conservation law without changing the results in any essential way.

The first condition in Eq. (2.17) is energy conservation; the next is inserted because exchange of equivalent spins has no effect; the third condition limits the interchanges to next-nearest-neighbor sites. The condition of energy conservation can be restated with the aid of Eq. (2.11b) as

$$u_{\mathbf{r}}=u_{\mathbf{r}'}. \tag{2.18}$$

Here $u_{\mathbf{r}}$ is the "potential energy" for a spin at site $\mathbf{r}$,

$$u_{\mathbf{r}}=\sum_{\mathbf{r}'\supset\mathbf{r}}\sigma_{\mathbf{r}'}. \tag{2.19}$$

The notation $\mathbf{r}'\supset\mathbf{r}$ indicates that the sum covers those values of $\mathbf{r}'$ which are nearest neighbors to $\mathbf{r}$. Thus the "energy conserving" operator $\Delta_{\mathbf{r},\mathbf{r}'}{}^{A}$ can be written as

$$\Delta_{\mathbf{r},\mathbf{r}'}{}^{A}=\delta(u_{\mathbf{r}},u_{\mathbf{r}'})\tfrac{1}{2}(1-\sigma_{\mathbf{r}}\sigma_{\mathbf{r}'}), \tag{2.20}$$

when $\mathbf{r}$ and $\mathbf{r}'$ are next-nearest neighbors.

Notice that the transition matrix (2.14) contains two terms. These terms are best understood if we return to the $p_{\alpha's}$. Equation (2.14) indicates a contribution to dp_α/dt which is

$$\sum_\beta w^A(\mathbf{I}_{\mathbf{r},\mathbf{r}'})_{\alpha\beta}(\Delta_{\mathbf{r},\mathbf{r}'}{}^{A})_\beta p_\beta(t)-w^A(\Delta_{\mathbf{r},\mathbf{r}'}{}^{A})_\alpha p_\alpha(t).$$

The first term, the "scattering-in term" indicates an increase in $p_\alpha(t)$ resulting from the scattering from all other states, β, into the state α. The second term, the "scattering-out term" shows the decrease in $p_\alpha(t)$ coming from the scattering out of that state. The projection operators $\Delta_{\mathbf{r},\mathbf{r}'}$ simply delimit the states in which the scattering is permitted.

The model we have just defined satisfies all the formal requirements described in Sec. (2A). Since $\langle\,|$ contains all states equally,

$$\langle\,|\,\mathbf{I}_{\mathbf{r},\mathbf{r}'}=\langle\,|\,. \tag{2.21}$$

Hence the definition (2.14) automatically guarantees the detailed balancing condition (2.6) since

$$\langle\,|\,\mathbf{T}_{\mathbf{r},\mathbf{r}'}{}^{A}=\langle\,|\,(\mathbf{I}_{\mathbf{r},\mathbf{r}'}-1)\Delta_{\mathbf{r},\mathbf{r}'}{}^{A}w^A=0.$$

The conservation laws (2.12) for energy and magnetization are also automatically satisfied in this model. Since $\mathbf{I}_{\mathbf{r},\mathbf{r}'}$ only interchanges spins, it commutes with the total magnetization, $\sum_{\mathbf{r}}\sigma_{\mathbf{r}}$. Also, the projection operation which insists that $u_{\mathbf{r}}=u_{\mathbf{r}'}$ for all interchanges then guarantees that no interchange will change the value of the "Hamiltonian," $\mathbf{H}$.

C. Other Formal Requirements

We would like to demand that the equilibrium solution of the master equation be precisely the standard Ising-model density matrices

$$p_\alpha=\exp(-\beta H_\alpha+hM_\alpha)/Z, \tag{2.22a}$$

with

$$Z(\beta,h)=\sum_\alpha\exp(-\beta H_\alpha+hM_\alpha), \tag{2.22b}$$

where β is a dimensionless inverse temperature and h is a dimensionless magnetic field. This is the same as the requirement that the state

$$|eq\rangle=(1/Z(\beta,h))\exp(-\beta\mathbf{H}+h\mathbf{M})|\,\rangle \tag{2.23}$$

be a time-independent solution of the master equation. Since the master reads

$$(\partial/\partial t)|t\rangle=\mathbf{T}|t\rangle,$$

we must require

$$\mathbf{T}\exp(-\beta\mathbf{H}+h\mathbf{M})|\,\rangle=0.$$

But, the transition matrix $\mathbf{T}$ commutes with $\mathbf{H}$ and $\mathbf{M}$. The condition that Eq. (2.23) be an equilibrium solution is then the requirement

$$\mathbf{T}|\,\rangle=0. \tag{2.24}$$

Equation (2.23) is automatically satisfied in this simple model. For $\mathbf{I}_{\mathbf{r},\mathbf{r}'}$ commutes with $\Delta_{\mathbf{r},\mathbf{r}'}$ so that

$$\mathbf{T}_{\mathbf{r},\mathbf{r}'}{}^{A}=\Delta_{\mathbf{r},\mathbf{r}'}{}^{A}(\mathbf{I}_{\mathbf{r},\mathbf{r}'}-1)w^A.$$

Then, $\mathbf{I}_{\mathbf{r},\mathbf{r}'}|\,\rangle=|\,\rangle$ implies

$$\mathbf{T}_{\mathbf{r},\mathbf{r}'}{}^{A}|\,\rangle=0.$$

Below, we shall consider another model in which $\mathbf{I}_{\mathbf{r},\mathbf{r}'}$ does not commute with $\Delta_{\mathbf{r},\mathbf{r}'}$. In this situation, there will be real difficulty in constructing a model with the correct equilibrium properties.

Notice the structure of the matrix $\mathbf{T}$. It has the form

$$T_{\alpha\beta}=(\mathbf{T}^{\text{in}})_{\alpha\beta}-\delta_{\alpha\beta}T_\alpha{}^{\text{out}}. \tag{2.25}$$

The first term in $\mathbf{T}$ comes from the "scattering in" term in each of the $\mathbf{T}_{\mathbf{r},\mathbf{r}'}$. Since these terms are all proportional to $\mathbf{I}_{\mathbf{r},\mathbf{r}'}\frac{1}{2}(1-\sigma_{\mathbf{r}}\sigma_{\mathbf{r}'})$, they are completely off diagonal. Furthermore, they are positive semidefinite, i.e.,

$$\begin{aligned}&T_{\alpha\beta}{}^{\text{in}}\geqslant 0,\\ &T_{\alpha\alpha}{}^{\text{in}}=0.\end{aligned} \tag{2.26}$$

Also, the detailed balancing condition requires$\langle\,|\,\mathbf{T}=0$, or

$$T_\beta{}^{\text{out}}=\sum_\alpha T_{\alpha\beta}{}^{\text{in}}, \tag{2.27a}$$

while the statement that we have a correct equilibrium solution $\mathbf{T}|\,\rangle=0$ insures

$$T_\alpha{}^{\text{out}}=\sum_\beta T_{\alpha\beta}{}^{\text{in}}. \tag{2.27b}$$

In the model we have just described Eqs. (2.27a) and (2.27b) are essentially identical, because $T_{\alpha\beta}$ is a symmetrical matrix. However, below we shall consider

a T matrix which is not symmetrical but nonetheless satisfies both (2.27a) and (2.27b).

D. Eigenstates of T

Let the matrix $\mathbf{T}$ have the eigenstate $|\nu\rangle$ such that

$$\mathbf{T}|\nu\rangle=-s_\nu|\nu\rangle, \tag{2.28}$$

so that s_ν is an eigenvalue of $-\mathbf{T}$. If a state $|t\rangle$ is a superposition of such eigenstates

$$|t\rangle=\sum_\nu a_\nu(t)|\nu\rangle,$$

then the equation of motion

$$(\partial/\partial t)|t\rangle=\mathbf{T}|t\rangle$$

implies that

$$a_\nu(t)=e^{-s_\nu t}a_\nu(0). \tag{2.29}$$

The stability of the system demands that exponentials in Eq. (2.29) never become infinite. This is equivalent to the statement

$$\mathrm{Re}s_\nu\geqslant 0 \tag{2.30a}$$

or

$$\mathrm{Re}\langle\nu|\mathbf{T}|\nu\rangle\leqslant 0. \tag{2.30b}$$

In our specific example, $\mathbf{T}^A$ is a Hermitian operator since $\mathbf{I}_{\mathbf{r},\mathbf{r}'}$ commutes with $\Delta_{\mathbf{r}\mathbf{r}'}$. This Hermiticity guarantees that all the eigenvalues s_ν are real. Later on we shall consider a non-Hermitian $\mathbf{T}$. However, Eqs. (2.30) must be equally true whether or not $\mathbf{T}$ is Hermitian.

To see this point, write the eigenstate $|\nu\rangle$ as

$$|\nu\rangle=\sum_\alpha a_\alpha|\alpha\rangle,$$
$$\langle\nu|=\sum_\alpha\langle\alpha|a_\alpha{}^*. \tag{2.31}$$

If $|\nu\rangle$ is properly normalized

$$\begin{aligned}2\,\mathrm{Re}s_\nu&=-2\,\mathrm{Re}\langle\nu|\mathbf{T}|\nu\rangle\\&=-2\,\mathrm{Re}\sum_{\alpha\beta}T_{\alpha\beta}a_\alpha{}^*a_\beta\\&=-\sum_{\alpha\beta}T_{\alpha\beta}(a_\alpha{}^*a_\beta+a_\alpha a_\beta{}^*).\end{aligned}$$

The last line follows because $T_{\alpha\beta}$ is real. Equations (2.25) and (2.27) now give

$$2\,\mathrm{Re}s_\nu=\sum_{\alpha\beta}T_{\alpha\beta}{}^{\mathrm{in}}|a_\alpha-a_\beta{}^*|^2. \tag{2.32}$$

The desired result, Eq. (2.30a), follows immediately from the fact that $T_{\alpha\beta}{}^{\mathrm{in}}\geqslant 0$.

III. ANALYSIS OF HERMITIAN TRANSPORT MODEL

In this section, we analyze the transport properties of the model introduced in Sec. 2.2.

A. Conservation Laws and Currents

The two conserved operators, $\mathbf{M}$ and $\mathbf{H}$, are sums over all sites of a magnetization density operator and an energy density

$$\begin{aligned}m(\mathbf{r})&=\sigma_\mathbf{r}-\langle\langle\sigma_\mathbf{r}\rangle\rangle,\\ \epsilon(\mathbf{r})&=-\tfrac{1}{2}u_\mathbf{r}\sigma_\mathbf{r}+\langle\langle\tfrac{1}{2}u_\mathbf{r}\sigma_\mathbf{r}\rangle\rangle.\end{aligned} \tag{3.1}$$

The double bracket indicates an equilibrium average in the Ising model and

$$u(\mathbf{r})=\sum_{\mathbf{r}'\supset\mathbf{r}}\sigma_{\mathbf{r}'}. \tag{3.2}$$

These two densities obey local conservation laws

$$\begin{aligned}(\partial/\partial t)\langle\,|m(\mathbf{r})|\,t\rangle+\nabla\cdot\langle\,|\mathbf{j}^m(\mathbf{r})|\,t\rangle&=0,\\ (\partial/\partial t)\langle\,|\epsilon(\mathbf{r})|\,t\rangle+\nabla\cdot\langle\,|\mathbf{j}^\epsilon(\mathbf{r})|\,t\rangle&=0.\end{aligned} \tag{3.3}$$

To find the currents we make use of the master equation. For example,

$$\nabla\cdot\langle\,|\mathbf{j}^m(\mathbf{r})|\,t\rangle=-\langle\,|m(\mathbf{r})\mathbf{T}|\,t\rangle, \tag{3.4}$$

so that

$$\begin{aligned}\nabla\cdot\langle\,|\mathbf{j}^m(\mathbf{r})&=\langle\,|[\mathbf{T},\sigma_\mathbf{r}]\\&=\tfrac{1}{2}w^A\sum_{\mathbf{r}'\mathbf{r}''}\langle\,|[(\mathbf{I}_{\mathbf{r}',\mathbf{r}''}-1),\sigma_\mathbf{r}]\Delta_{\mathbf{r}',\mathbf{r}''}{}^A\\&=w^A\sum_{\mathbf{r}'}\langle\,|[\mathbf{I}_{\mathbf{r},\mathbf{r}'},\sigma_\mathbf{r}]\Delta_{\mathbf{r}',\mathbf{r}}{}^A\\&=w^A\sum_{\mathbf{r}'}\langle\,|(\sigma_\mathbf{r}-\mathbf{I}_{\mathbf{r},\mathbf{r}'}\sigma_\mathbf{r}\mathbf{I}_{\mathbf{r},\mathbf{r}'})\Delta_{\mathbf{r},\mathbf{r}'}{}^A.\end{aligned}$$

The line of argument follows because $\langle\,|$ is an eigenstate of $\mathbf{I}_{\mathbf{r},\mathbf{r}'}$ with eigenvalue unity and also because $\mathbf{I}_{\mathbf{r},\mathbf{r}'}$ commutes with $\Delta_{\mathbf{r},\mathbf{r}'}{}^A$. Since $\mathbf{I}_{\mathbf{r},\mathbf{r}'}$ converts $\sigma_\mathbf{r}$ into $\sigma_{\mathbf{r}'}$ we find

$$\nabla\cdot\mathbf{j}^m(r)=w^A\sum_{\mathbf{r}'}\Delta_{\mathbf{r},\mathbf{r}'}{}^A(\sigma_\mathbf{r}-\sigma_{\mathbf{r}'}). \tag{3.5}$$

To eliminate the divergence in Eq. (3.5) multiply by $e^{-i\mathbf{q}\cdot\mathbf{r}}$ and sum over all $\mathbf{r}$.

Then,

$$\sum_\mathbf{r}i\mathbf{q}\cdot\mathbf{j}^m(r)e^{-i\mathbf{q}\cdot\mathbf{r}}=\tfrac{1}{2}\sum_{\mathbf{r},\mathbf{r}'}(e^{-i\mathbf{q}\cdot\mathbf{r}}-e^{-i\mathbf{q}\cdot\mathbf{r}'})w^A\Delta_{\mathbf{r},\mathbf{r}'}{}^A(\sigma_\mathbf{r}-\sigma_{\mathbf{r}'}).$$

For small q, the difference of exponentials reduces to $i\mathbf{q}\cdot(\mathbf{r}'-\mathbf{r})e^{-i\mathbf{q}\cdot\mathbf{r}}$. An inversion of the Fourier transform then gives

$$\mathbf{j}^m(\mathbf{r})=w^A\sum_{\mathbf{r}'}(\mathbf{r}'-\mathbf{r})\Delta_{\mathbf{r},\mathbf{r}'}{}^A\tfrac{1}{2}(\sigma_\mathbf{r}-\sigma_{\mathbf{r}'}). \tag{3.6}$$

A similar but slightly more complex calculation gives a form for the energy current.

B. Local Equilibrium Solution

Equations (3.3) are exact local conservation laws. However, these conservation laws cannot be used

without a solution for the nonequilibrium state of the system. We follow Kawasaki[1] in employing a local equilibrium approximation in which the nonequilibrium state is approximated by

$$|t\rangle = -\sum_{\mathbf{r}} [\delta\beta(\mathbf{r},t)\epsilon(\mathbf{r}) - \delta h(\mathbf{r},t)m(\mathbf{r})]|eq\rangle. \quad (3.7)$$

In Eq. (3.7), $\delta\beta(\mathbf{r},t)$ and $\delta h(\mathbf{r},t)$ have the physical significance of being the local deviation of inverse temperature and magnetic field from their equilibrium values.

We employ (3.7) as an approximate eigenstate of T. The low-lying eigenstates of T determine the slow relaxation toward equilibrium which is characteristic of transport processes. In particular, the two smallest eigenvalues of $-\mathsf{T}$ for small q are

$$s_1 = D_s q^2,$$
$$s_2 = D_T q^2, \quad (3.8)$$

where D_s and D_T are the spin and thermal diffusivities.

To find approximate eigenvalues of T, we assume that the disturbance has wave vector $\mathbf{q}$ and eigenvalue s. The n, $|t\rangle$ can be written as

$$|t\rangle = p_{eq}e^{-st}[\,|m,\mathbf{q}\rangle\delta h - |\epsilon,\mathbf{q}\rangle\delta\beta].$$

Here we have taken (3.9)

$$\delta h(\mathbf{r},t) = (1/\sqrt{N})e^{i\mathbf{q}\cdot\mathbf{r}-st}\delta h,$$

and written

$$|m,\mathbf{q}\rangle = (1/\sqrt{N})\sum_{\mathbf{r}} e^{i\mathbf{q}\cdot\mathbf{r}}m(\mathbf{r})\,|\,\rangle,$$
$$|\epsilon,\mathbf{q}\rangle = (1/\sqrt{N})\sum_{\mathbf{r}} e^{i\mathbf{q}\cdot\mathbf{r}}\epsilon(\mathbf{r})\,|\,\rangle. \quad (3.10)$$

N is the number of sites and p_{eq} is the equilibrium density matrix. The master equation now reads

$$-sp_{eq}[\,|m,\mathbf{q}\rangle\delta h - |\epsilon,\mathbf{q}\rangle\delta\beta] = \mathsf{T}p_{eq}[\,|m,\mathbf{q}\rangle\delta h - |\epsilon,\mathbf{q}\rangle\delta\beta]. \quad (3.11)$$

To form the local spin conservation law, we multiply this equation on the left by $\langle m,\mathbf{q}|$; to form the energy conservation law, we multiply by $\langle\epsilon,\mathbf{q}|$. The results of this multiplication are the pair of equations

$$-s[\chi_{mm}\delta h - \chi_{m\epsilon}\delta\beta] = -q^2[\lambda_{mm}\delta h - \lambda_{\epsilon m}\delta\beta]$$
$$-s[-\chi_{\epsilon m}\delta h + \chi_{\epsilon\epsilon}\delta\beta] = -q^2[-\lambda_{m\epsilon}\delta h + \lambda_{\epsilon\epsilon}\delta\beta], \quad (3.12)$$

where

$$\chi_{mm} = \langle m,\mathbf{q}|\,p_{eq}|\,m,\mathbf{q}\rangle,$$
$$-q^2\lambda_{mm} = \langle m,\mathbf{q}|\,\mathsf{T}p_{eq}|\,m,\mathbf{q}\rangle. \quad (3.13)$$

Equations (3.12) have a direct physical significance. The left-hand side of the first of these equations gives the time derivative of the magnetization produced by a magnetic field variation δh and an inverse temperature variation $\delta\beta$. The χ's are all thermodynamic derivatives. For example,

$$\chi_{mm} = (1/N)\sum_{\mathbf{r},\mathbf{r}'} e^{i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')}\langle\langle(\sigma_{\mathbf{r}} - \langle\langle\sigma\rangle\rangle)(\sigma_{\mathbf{r}'} - \langle\langle\sigma\rangle\rangle)\rangle\rangle$$

is just a dimensionless version of the ordinary spin susceptibility as calculated from the equilibrium behavior of the ordinary Ising model. Similarly, $\chi_{\epsilon\epsilon}$ is the specific heat and $\chi_{m\epsilon}$ the derivative of the magnetization with respect to temperature. All these thermodynamic derivatives diverge near the critical point.

The right-hand side of Eq. (3.12) gives the divergence of the currents in the presence of the gradients of magnetic field and temperature. Hence, the λ's are the transport coefficients of the model as determined by our local equilibrium approximation. For example, $\lambda_{\epsilon\epsilon}$ is the thermal conductivity, λ_{mm} is the spin-diffusion transport coefficient.

It is relatively easy to calculate the transport coefficients in this local equilibrium approximation. For example, the spin-diffusion coefficient is given by

$$-q^2\lambda_{mm} = (w^A/2N)\sum_{\mathbf{r}_1,\mathbf{r}_2}\sum_{\mathbf{r},\mathbf{r}'} e^{-i\mathbf{q}\cdot(\mathbf{r}_1-\mathbf{r}_2)} \times\langle\,|\sigma_{\mathbf{r}_1}\Delta_{\mathbf{r},\mathbf{r}'}{}^A(\mathbf{l}_{\mathbf{r},\mathbf{r}'} - \mathbf{1})\sigma_{\mathbf{r}_2}|eq\rangle.$$

In the sums over $\mathbf{r}_1$ and $\mathbf{r}_2$, the only nonvanishing terms are those with

$$\mathbf{r}_1 = \mathbf{r} \text{ or } \mathbf{r}',$$
$$\mathbf{r}_2 = \mathbf{r} \text{ or } \mathbf{r}'.$$

Since $\sigma_{\mathbf{r}} = -\sigma_{\mathbf{r}'}$, the expression simplifies to

$$-q^2\lambda_{mm} = (w^A/N)\sum_{\mathbf{r},\mathbf{r}'} 2[1-\cos\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')]\langle\,|\Delta_{\mathbf{r},\mathbf{r}'}{}^A|eq\rangle.$$

For small q we may expand the cosine and find

$$\lambda_{mm} = (w^A/N)\sum_{\mathbf{r},\mathbf{r}'} (x-x')^2\langle\langle\Delta_{\mathbf{r},\mathbf{r}'}{}^A\rangle\rangle.$$

In three dimensions we find

$$\lambda_{mm} = 8w^A\langle\langle\tfrac{1}{2}(1-\sigma_{\mathbf{r}}\sigma_{\mathbf{r}'})\delta(u_{\mathbf{r}},u_{\mathbf{r}'})\rangle\rangle, \quad (3.14a)$$

where $\mathbf{r}$ and $\mathbf{r}'$ are any pair of next-nearest neighbors. Similar calculations give

$$\lambda_{m\epsilon} = \lambda_{\epsilon m} = 4(-\tfrac{1}{2})w^A \times\langle\langle(u_{\mathbf{r}}+2v_{\mathbf{r}})\tfrac{1}{2}(1-\sigma_{\mathbf{r}}\sigma_{\mathbf{r}'})\delta(u_{\mathbf{r}},u_{\mathbf{r}'})\rangle\rangle, \quad (3.14b)$$

where $u_{\mathbf{r}}$ is defined in Eq. (2.19) and $v_{\mathbf{r}}$ is the sum of all nearest-neighbor spins of $\mathbf{r}$ which are not also nearest-neighbor spins of $\mathbf{r}'$ and

$$\lambda_{\epsilon\epsilon} = 4(\tfrac{1}{2})^2w^A\langle\langle[(u_{\mathbf{r}}+2v_{\mathbf{r}})^2 + (\sigma_{\mathbf{r}-\hat{e}_x} - \sigma_{\mathbf{r}'+\hat{e}_y})^2] \times\tfrac{1}{2}(1-\sigma_{\mathbf{r}}\sigma_{\mathbf{r}'})\delta(u_{\mathbf{r}},u_{\mathbf{r}'})\rangle\rangle, \quad (3.14c)$$

where $\hat{e}_x$ and $\hat{e}_y$ are unit vectors in the x and y directions respectively. Equations (3.14b) and (3.14c) are given for two dimensions since the expressions are slightly more complicated in three dimensions due to the greater number of nonequivalent nearest neighbors.

The significant feature of the results (3.14) is that the transport coefficients, λ, are all finite even at the critical point. This follows because $\Delta_{r,r'}$ and the σ's are all bounded operators. Therefore, this local equilibrium approximation gives all transport coefficients finite values.

To determine the relaxation rate spectrum, one would have to find the eigenvalues, s_1 and s_2, of the Eqs. (3.12). There is one particularly simple case. If the magnetic field is zero and the temperature is above the critical temperature, there is complete symmetry between spin up and spin down. Then $\chi_{m\epsilon}$ and $\lambda_{m\epsilon}$ both vanish so that Eqs. (3.12) become

$$-s\chi_{mm}\delta h=-q^2\lambda_{mm}\delta h\,,$$
$$-s\chi_{\epsilon\epsilon}\delta\beta=-q^2\lambda_{\epsilon\epsilon}\delta\beta. \tag{3.15}$$

Equations (3.15) indicate a diffusive type relaxation with diffusivities

$$D_s=\lambda_{mm}/\chi_{mm}\,,$$
$$D_T=\lambda_{\epsilon\epsilon}/\chi_{\epsilon\epsilon}. \tag{3.16}$$

Therefore, this local equilibrium approximation implies that the spin diffusivity D_s goes to zero as the inverse spin susceptibility near the critical point, while the thermal diffusivity, D_T, vanishes as the inverse specific heat.

C. Variational Statements

As Kawasaki[2] pointed out, the approximate evaluations of the transport coefficients as given by Eq. (3.13) are particularly significant, because there exist variational statements which indicate that these results are in some cases upper bounds on the coefficients.

Consider, in particular, the case $T>T_c$ and $h=0$. In that case, we have determined two approximate eigenvalues of $-\mathbf{T}$,

$$s_1^{\text{approx}}=\lambda_{mm}q^2/\chi_{mm} \tag{3.17a}$$

and

$$s_2^{\text{approx}}=\lambda_{\epsilon\epsilon}q^2/\chi_{\epsilon\epsilon} \tag{3.17b}$$

for small q. Here λ_{mm} and $\lambda_{\epsilon\epsilon}$ are given by Eqs. (3.14).

We claim that the exact transport coefficients will be smaller than these approximate coefficients. The exact coefficients, λ_T= thermal conductivity and λ_s= spin-diffusion transport coefficient, may be defined in terms of the smallest eigenvalues of $-\mathbf{T}$ for wave vector q. These eigenvalues are

$$s_1=\lambda_s q^2/\chi_{mm}\,,$$
$$s_2=\lambda_T q^2/\chi_{\epsilon\epsilon}\,, \tag{3.18}$$

where the χ's are the spin-susceptibility and the specific heat.

Equations (3.18) describe a slow, diffusive decay of long wavelength excitations. This slow decay occurs because $\mathbf{T}$ has a pair of eigenvalues which go to zero as q goes to zero. In fact, there are many such eigenvalues corresponding to different values of the equilibrium temperature and magnetic field. However, in any situation of small deviations from equilibrium at a given temperature and field, only two eigenvalues will count—all the eigenvalues corresponding to different equilibrium parameters will have zero weight.[17]

The two exact eigenvalues correspond to eigenstates $|1,\mathbf{q}\rangle$ and $|2,\mathbf{q}\rangle$ which obey

$$s_\nu p_{eq}|\nu,q\rangle=-\mathbf{T}p_{eq}|\nu,q\rangle \quad (\nu=1,2). \tag{3.19}$$

The eigenstates are normalized so that

$$\langle\nu,\mathbf{q}|\,p_{eq}|\nu,\mathbf{q}\rangle=1. \tag{3.20}$$

The requirement that you cannot go too far away from the equilibrium state for the given value of β and h can be stated as the demand that $|\nu,\mathbf{q}\rangle$ be a sum of quasi-local operators times $|\ \rangle$.

Since $-\mathbf{T}$ is Hermitian and $|1,\mathbf{q}\rangle$ is the lowest eigenvalue with wave vector $\mathbf{q}$,

$$s_1\leqslant\langle x,\mathbf{q}|\,(-\mathbf{T})p_{eq}|x,\mathbf{q}\rangle/\langle x,\mathbf{q}|\,p_{eq}|x,\mathbf{q}\rangle\,, \tag{3.21}$$

where $|x,\mathbf{q}\rangle$ is any state with wave vector $\mathbf{q}$. In our calculation, we used as an approximate eigenstate

$$|m,\mathbf{q}\rangle=\frac{1}{(\chi_{mm}N)^{1/2}}\sum_{\mathbf{r}}e^{i\mathbf{q}\cdot\mathbf{r}}m(\mathbf{r})|\ \rangle.$$

With this approximate state, the right-hand side of Eq. (3.21) becomes $\lambda_{mm}q^2/\chi_{mm}$. Therefore, it follows that

$$s_1\leqslant\lambda_{mm}q^2/\chi_{mm}.$$

Equation (3.18) then indicates that the exact spin-diffusion transport coefficient obeys

$$\lambda_s\leqslant\lambda_{mm}. \tag{3.22}$$

Hence this transport coefficient cannot diverge.

The exact spin-diffusion state has, for $h=0$ and temperatures above T_c, odd parity under an operation in which all spins flip sign. The thermal conduction eigenstate has even parity under this operation. Since $\mathbf{T}$ commutes with this spin-parity operation, there exist separate variational principles for the lowest eigenstates of even and odd parity. The lowest even-parity state of $-\mathbf{T}$ has eigenvalue $D_T^{\text{exact}}q^2$. The variational principle for the lowest exact even-parity state gives the fact that

$$\lambda_T\leqslant\lambda_{\epsilon\epsilon}\,, \tag{3.23}$$

where λ_T is the exact thermal conductivity and $\lambda_{\epsilon\epsilon}$ is our approximate conductivity.

The statement (3.22) holds for all temperatures and magnetic fields. However, Eq. (3.23) requires the spin-parity symmetry which only holds for $h=0$ and tem-

[17] R. Haag, N. M. Hugenholtz, and M. Winnink in an unpublished report have discussed how the apparent temperature dependence of eigenvalues may arise in many a particle system.

peratures above the critical temperature. Notice that both variational statements are only valid because $-\mathbf{T}$ is Hermitian.

IV. ANALYSIS OF A MODEL WHICH INCLUDES SOUND WAVES

The last chapter discussed a model with a Hermitian $\mathbf{T}$. Now, we turn to a model rich enough to include sound waves. In this case, we must have eigenvalues of $-\mathbf{T}$ given by $s_\nu(q)=\pm icq$ where c is the sound velocity and i is $\sqrt{-1}$. Clearly, we must abandon any hope of a Hermitian $\mathbf{T}$ at this point. Hermitian $\mathbf{T}$'s cannot give the imaginary eigenvalues which are the hallmark of sound waves.

A. A Model Which Includes Sound Waves

In this section we describe a model which has sound waves among its nonequilibrium modes and has as its equilibrium solution an Ising model.

Again in this model we consider a three-dimensional cubic lattice with N sites. There is again a spin variable, $\sigma_\mathbf{r}=\pm 1$, for each site. In addition, there is a vector variable, a "momentum," for each site. For a two-dimensional lattice, $\mathbf{g}_\mathbf{r}$ has the values

$$\begin{aligned}&\mathbf{g}_\mathbf{r}=0 \quad \text{if} \quad \sigma_\mathbf{r}=-1,\\ &\mathbf{g}_\mathbf{r}=(1,1),\ (1,-1),\ (-1,1) \text{ or } (-1,-1)\\ &\qquad\qquad\qquad\qquad \text{if} \quad \sigma_\mathbf{r}=+1,\end{aligned} \tag{4.1a}$$

while for a three dimensional lattice

$$\begin{aligned}&\mathbf{g}_\mathbf{r}=0 \quad \text{if} \quad \sigma_\mathbf{r}=-1,\\ &\mathbf{g}_\mathbf{r}=(1,1,0),\ (1,-1,0),\ (-1,1,0),\ (-1,-1,0),\\ &\quad (1,0,1),\ (1,0,-1),\ (-1,0,1),\ (-1,0,-1),\\ &\quad (0,1,1),\ (0,-1,1),\ (0,1,-1),\ \text{or } (0,-1,-1)\\ &\qquad\qquad\qquad\qquad \text{for} \quad \sigma_\mathbf{r}=+1,\end{aligned}$$

where $\mathbf{g}_\mathbf{r}$ in the "momentum" of a particle at the site $\mathbf{r}$.

A basis "state" of the system, $|\alpha\rangle$, will then be given by specifying all the spin variables and all the momentum variables.

It will be demanded that in this model the following quantities by conserved quantities:

$$\mathbf{N}=\sum_\mathbf{r} \tfrac{1}{2}(1+\sigma_\mathbf{r}) \tag{4.2a}$$

$$\mathbf{H}=-\sum_{\langle \mathbf{r},\mathbf{r}'\rangle} \sigma_\mathbf{r}\sigma_{\mathbf{r}'}, \tag{4.2b}$$

$$\mathbf{G}=\sum_\mathbf{r} \mathbf{g}_\mathbf{r}. \tag{4.2c}$$

$\mathbf{N}$ is called the number operator, $\mathbf{G}$ the total "momentum" operator, and $\mathbf{H}$ is the Hamiltonian. In view of the well-known connection between the lattice gas model of a fluid and the Ising model,[18,19] $\frac{1}{2}(1+\sigma_\mathbf{r})$ can be thought of as the density of the lattice gas at the site $\mathbf{r}$ so that $\sum_\mathbf{r}\sigma_\mathbf{r}=2\times$ (number of gas atoms)$+$constant—hence the terminology employed above. If there is no particle present $\sigma_\mathbf{r}=-1$. In that case, we have chosen to say that there is no momentum at the site. The momentum variable is chosen to be discrete in order to simplify the calculations. This discreteness may be a serious defect of the model.

Since $\mathbf{N}$, $\mathbf{H}$, and $\mathbf{G}$ are all conserved an appropriate equilibrium state will be

$$|eq.\rangle=\exp(-\beta\mathbf{H}+\mu\mathbf{N}+\mathbf{v}\cdot\mathbf{G})|\ \rangle/Z(\beta,\mu,\mathbf{v}), \tag{4.3}$$

with

$$Z(\beta,\mu,\mathbf{v})=\langle\ |\exp(-\beta\mathbf{H}+\mu\mathbf{N}+\mathbf{v}\cdot\mathbf{G})|\ \rangle.$$

Here β is a dimensionless inverse temperature, μ a dimensionless chemical potential, and $\mathbf{v}$ a dimensionless velocity. At $\mathbf{v}=\mathbf{0}$, in two dimensions the state $\sigma_\mathbf{r}=+1$ is four times as likely as the state $\sigma_\mathbf{r}=-1$. Hence the critical value of the chemical potential is defined by

$$4e^{\mu_c}=1 \tag{4.4}$$

for the two dimensional case. At $\mathbf{v}=\mathbf{0}$, Z differs from the Ising-model partition function by only a multiplicative factor. The Ising-model variable h, which is the dimensionless magnetic field, is related to μ by $h=\mu-\mu_c$.

We once again make use of a master equation of the form

$$(d/dt)|t\rangle=\mathbf{T}|t\rangle. \tag{4.5}$$

Here the state $|t\rangle$ is of the form

$$|t\rangle=\sum_\alpha p_\alpha(t)|\alpha\rangle,$$

where the index α defines the values of both spin and momentum at each site.

$\mathbf{T}$ must satisfy the general requirements given in Sec. II of this paper and commute with $\mathbf{N}$, $\mathbf{H}$, and $\mathbf{G}$. A $\mathbf{T}$ meeting all these requirements is

$$\mathbf{T}=\mathbf{T}^A+\mathbf{T}^B+\mathbf{T}^C. \tag{4.6}$$

Here $\mathbf{T}^A$ is the matrix described in the previous section. It describes processes in which particles fall into holes at next-nearest-neighbor sites. The next term, $\mathbf{T}^B$, has a very similar structure to $\mathbf{T}^A$:

$$\mathbf{T}^A=\tfrac{1}{2}w^A\sum_{\mathbf{r},\mathbf{r}'}(\mathbf{I}_{\mathbf{r},\mathbf{r}'}-1)\Delta_{\mathbf{r},\mathbf{r}'}{}^A, \tag{4.7a}$$

$$\mathbf{T}^B=w^B\sum_{\mathbf{r},\mathbf{r}'}(\mathbf{I}_{\mathbf{r},\mathbf{r}'}-1)\Delta_{\mathbf{r},\mathbf{r}'}{}^B. \tag{4.7b}$$

Now $\mathbf{I}_{\mathbf{r},\mathbf{r}'}$ is an interchange matrix which interchanges both the spin and the momentum at $\mathbf{r}$ and $\mathbf{r}'$. In

[18] T. D. Lee and C. N. Yang, Phys. Rev. 87, 410 (1952).
[19] K. Huang, *Statistical Mechanics* (John Wiley & Sons, Inc., N. Y., 1963).

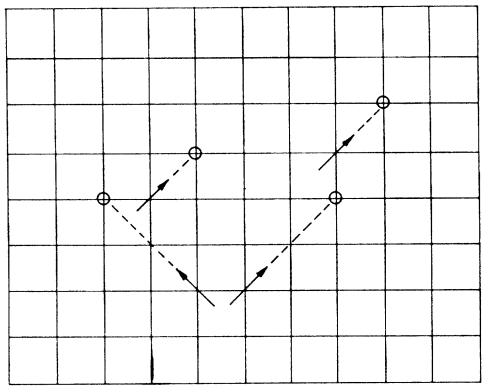


FIG. 2. Some allowed transitions for the T^B transition matrix. The particles momenta are denoted by the arrows and holes by unmarked intersections. The particles interchange with the circled holes lying on the line determined by particles momenta; the circled holes being the first holes for which an exchange is energetically allowed.

particular

$$\begin{aligned}
&\mathbf{I}_{\mathbf{r},\mathbf{r}'}\sigma_{\mathbf{r}}=\sigma_{\mathbf{r}'}\mathbf{I}_{\mathbf{r},\mathbf{r}'}\,,\\
&\mathbf{I}_{\mathbf{r},\mathbf{r}'}\mathbf{g}_{\mathbf{r}}=\mathbf{g}_{\mathbf{r}'}\mathbf{I}_{\mathbf{r},\mathbf{r}'}\,,\\
&[\mathbf{I}_{\mathbf{r},\mathbf{r}'},\sigma_{\mathbf{r}''}]=0 \quad \text{for} \quad \mathbf{r}''\neq\mathbf{r} \text{ or } \mathbf{r}'\,,\\
&[\mathbf{I}_{\mathbf{r},\mathbf{r}'},\mathbf{g}_{\mathbf{r}''}]=0 \quad \text{for} \quad \mathbf{r}''\neq\mathbf{r} \text{ or } \mathbf{r}'\,,\\
&\mathbf{I}_{\mathbf{r},\mathbf{r}'}=\mathbf{I}_{\mathbf{r}'\mathbf{r}}\,,\\
&(\mathbf{I}_{\mathbf{r},\mathbf{r}'})^2=\mathbf{1}.
\end{aligned} \tag{4.8}$$

In Eq. (4.7a) $\Delta_{\mathbf{r},\mathbf{r}'}{}^A$ is the same diagonal matrix as defined in Eq. (2.17). Therefore, the term $\mathbf{T}^A$ describes once again the diffusion of particles onto neighboring unoccupied sites.

Notice that this diffusion does not depend upon the momentum of the particle. The transition matrix, $\mathbf{T}^B$, introduces the momentum. Physically, we want a particle to move in the direction of its momentum and land in the first unoccupied site which is permissible from the point of view of energy conservation. The projection operator $\Delta_{\mathbf{r},\mathbf{r}'}{}^B$ in Eq. (4.7b) is designed to produce a proper operator for describing the motion of a particle from $\mathbf{r}$ to $\mathbf{r}'$. We write

$$\Delta_{\mathbf{r},\mathbf{r}'}{}^B=1 \quad \text{if}$$

(a) $\sigma_{\mathbf{r}}=+1 \quad \sigma_{\mathbf{r}'}=-1 \quad u_{\mathbf{r}}=u_{\mathbf{r}'}$,

and (b) there is a positive integer n such that

$$\mathbf{r}+n\mathbf{g}_{\mathbf{r}}=\mathbf{r}'\,,$$

and (c) there is no site $\mathbf{r}'$ which satisfies conditions a and b for a smaller positive value of n.

Otherwise, $\Delta_{\mathbf{r},\mathbf{r}'}{}^B=0$. In symbols

$$\Delta_{\mathbf{r},\mathbf{r}'}{}^B=\tfrac{1}{2}(1+\sigma_{\mathbf{r}})\tfrac{1}{2}(1-\sigma_{\mathbf{r}'})\delta(u_{\mathbf{r}},u_{\mathbf{r}'})\times\sum_{n=1}^{\infty}\delta(\mathbf{r}+n\mathbf{g}_{\mathbf{r}},\mathbf{r}')\theta_{\mathbf{r},\mathbf{r}'}. \tag{4.9}$$

Here $\theta_{\mathbf{r},\mathbf{r}'}$ is the projection operator which enforces condition (c). It has the structure

$$\theta_{\mathbf{r},\mathbf{r}'}=\prod_{n''=1}^{n-1}(1-\delta(u_{\mathbf{r}},u_{\mathbf{r}+n''\mathbf{g}_{\mathbf{r}}}))\tfrac{1}{2}(1-\sigma_{\mathbf{r}+n''\mathbf{g}_{\mathbf{r}}}), \tag{4.10}$$

where $\mathbf{g}$ is a vector of length $\sqrt{2}$ pointing from $\mathbf{r}$ to $\mathbf{r}'$.

Some allowed and forbidden exchanges are shown in Fig. 2.

The whole point of this rather complex construction of $\Delta_{\mathbf{r},\mathbf{r}'}{}^B$ is to make sure that every particle has one and only one place to go. In symbols

$$\sum_{\mathbf{r}'}\Delta_{\mathbf{r},\mathbf{r}'}{}^B=\tfrac{1}{2}(1+\sigma_{\mathbf{r}}). \tag{4.11}$$

Equation (4.11) underlies the condition which allows the complicated transition matrix $\mathbf{T}^B$ to have an Ising-model equilibrium solution.

$\mathbf{T}^A$ was discussed in Sec. II of this paper so we know that it commutes with $\mathbf{N}$, $\mathbf{H}$, and $\mathbf{G}$, conserves probability and has the proper Ising-model equilibrium solution.

$\mathbf{T}^B$ is a more complicated object since $\mathbf{I}_{\mathbf{r},\mathbf{r}'}$ does not commute with $\Delta_{\mathbf{r},\mathbf{r}'}{}^B$. In fact, if we define

$$\mathbf{I}_{\mathbf{r},\mathbf{r}'}\Delta_{\mathbf{r},\mathbf{r}'}{}^B\mathbf{I}_{\mathbf{r},\mathbf{r}'}=\tilde{\Delta}_{\mathbf{r}',\mathbf{r}}{}^B, \tag{4.12}$$

we discover that

$$\tilde{\Delta}_{\mathbf{r},\mathbf{r}'}{}^B=\tfrac{1}{2}(1+\sigma_{\mathbf{r}})\tfrac{1}{2}(1-\sigma_{\mathbf{r}'})\delta(u_{\mathbf{r}},u_{\mathbf{r}'})\times\sum_{n=1}^{\infty}\delta(\mathbf{r}-n\mathbf{g}_{\mathbf{r}},\mathbf{r}')\theta_{\mathbf{r},\mathbf{r}'}. \tag{4.13}$$

Notice the minus sign in the term involving $\mathbf{g}_{\mathbf{r}}$ in Eq. (4.13). The same term is Eq. (4.9) has a plus sign. Hence $\tilde{\Delta}_{\mathbf{r},\mathbf{r}'}{}^B$ is different from $\Delta_{\mathbf{r},\mathbf{r}'}{}^B$. This difference means that $\mathbf{T}^B$ is not a Hermitian matrix—it is real but not symmetrical. In fact, not only is $\mathbf{T}^B$ not Hermitian but $\mathbf{T}^B$ is also not normal. That is, $\mathbf{T}^B$ does not commute with its adjoint which implies that $\mathbf{T}^B$ does not possess a complete set of orthonormal eigenvectors.

Physically, the difference between Δ and $\tilde{\Delta}$ arises because these functions answer different questions. When $\Delta_{\mathbf{r},\mathbf{r}'}{}^B=1$, a particle at $\mathbf{r}$ can go to $\mathbf{r}'$. Thus $\mathbf{g}_{\mathbf{r}}$ points from $\mathbf{r}$ to $\mathbf{r}'$. When $\Delta_{\mathbf{r},\mathbf{r}'}{}^B=1$, a particle at $\mathbf{r}$ *can have come from* $\mathbf{r}'$. Then $\mathbf{g}_{\mathbf{r}}$ must point from $\mathbf{r}'$ to $\mathbf{r}$.

Notice that every particle can come from one and only one place. This means that

$$\sum_{\mathbf{r}'}\tilde{\Delta}_{\mathbf{r},\mathbf{r}'}{}^B=\tfrac{1}{2}(1+\sigma_{\mathbf{r}}). \tag{4.14}$$

Notice that similarity between Eqs. (4.11) and (4.14). As a result of this symmetry, $\mathbf{T}^B$ has one important left-right symmetry property. According to Eqs. (4.7b)

and (4.12)

$$\mathbf{T}^B = w^B \sum_{\mathbf{r},\mathbf{r}'} (\mathbf{I}_{\mathbf{r},\mathbf{r}'} - \mathbf{1})\Delta_{\mathbf{r},\mathbf{r}'}{}^B$$

$$= w^B \sum_{\mathbf{r},\mathbf{r}'} [\tilde{\Delta}_{\mathbf{r}',\mathbf{r}}{}^B \mathbf{I}_{\mathbf{r},\mathbf{r}'} - \Delta_{\mathbf{r},\mathbf{r}'}{}^B]. \quad (4.15)$$

But, according to Eqs. (4.14) and (4.11) the last Δ^B in Eq. (4.15) can be replaced by $\tilde{\Delta}^B$. Hence,

$$\mathbf{T}^B = w^B \sum_{\mathbf{r},\mathbf{r}'} \tilde{\Delta}_{\mathbf{r},\mathbf{r}'}{}^B (\mathbf{I}_{\mathbf{r},\mathbf{r}'} - \mathbf{1}). \quad (4.16)$$

Equation (4.16) has the same structure as Eq. (4.7b)—only now the $\mathbf{I}$ appears on the right.

This structual similarity is quite important indeed. The form (4.7b) for $\mathbf{T}^B$ clearly indicates that

$$\langle\,|\,\mathbf{T}^B = 0,$$

so that $\mathbf{T}^B$ satisfies the detailed balancing condition. On the other hand, the form (4.16) is necessary in order to see that

$$\mathbf{T}^B|\,\rangle = 0.$$

This latter condition ensures that $\mathbf{T}^B$ has the correct Ising-model equilibrium solution.

Notice that $\mathbf{T}^A$ and $\mathbf{T}^B$ each conserve the total number of particles with a given value of $\mathbf{g}_\mathbf{r}$. These terms alone give too many "momentum" conservation laws. In order to mix different values of $\mathbf{g}_\mathbf{r}$ we introduce a scattering term

$$\mathbf{T}^C = \tfrac{1}{2} w^C \sum_{\mathbf{r},\mathbf{r}'} (\mathbf{J}_{\mathbf{r},\mathbf{r}'} - \mathbf{1}j)\Delta_{\mathbf{r},\mathbf{r}'}{}^C. \quad (4.17)$$

The term (4.17) is designed to allow isotropic scattering of nearest-neighbor particles if the total momentum of these particles is zero as depicted in Fig. 3. Hence

$$\Delta_{\mathbf{r},\mathbf{r}'}{}^C = \tfrac{1}{2}(1+\sigma_\mathbf{r})\tfrac{1}{2}(1-\sigma_{\mathbf{r}'})\delta(\mathbf{g}_\mathbf{r}+\mathbf{g}_{\mathbf{r}'},\mathbf{0}), \quad (4.18)$$

when $\mathbf{r}$ and $\mathbf{r}'$ are nearest neighbors. Otherwise $\Delta_{\mathbf{r},\mathbf{r}'}{}^C$ is zero. The operator $\mathbf{J}_{\mathbf{r},\mathbf{r}'}$ changes the values of $\mathbf{g}_\mathbf{r}$ and $\mathbf{g}_{\mathbf{r}'}$. In matrix notation

$$\langle \bar{\mathbf{g}}_\mathbf{r}, \bar{\mathbf{g}}_{\mathbf{r}'} | \mathbf{J}_{\mathbf{r},\mathbf{r}'} | \mathbf{g}_\mathbf{r}\mathbf{g}_{,\mathbf{r}'} \rangle = \delta(\bar{\mathbf{g}}_\mathbf{r}+\bar{\mathbf{g}}_{\mathbf{r}'},\mathbf{0})\delta(\mathbf{g}_\mathbf{r}+\mathbf{g}_{\mathbf{r}'},\mathbf{0}). \quad (4.18')$$

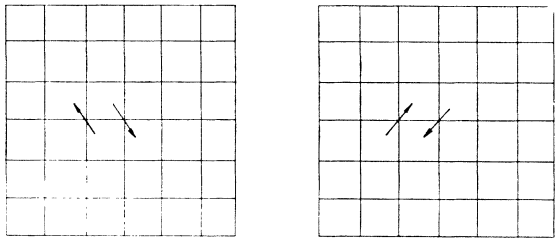
To ensure

$$\mathbf{T}^C|\,\rangle = \langle\,|\,\mathbf{T}^C = 0,$$

it is only necessary to choose

$$\begin{aligned} j &= 4 \quad \text{in two dimensions,} \\ j &= 12 \quad \text{in three dimensions.} \end{aligned} \quad (4.19)$$

The model of a liquid-gas phase transition we have just described has one very serious drawback: It has cubic (or square) symmetry rather than a complete rotational invariance. On the other hand, it has some very important virtues. Energy, momentum, and particle number are exactly conserved. These quantities can flow from one point to a neighboring point but they are never increased or decreased. Since the transport modes are crucially connected with these conservation laws, it is probably very important that they be included exactly rather than in an averaged sense.[1,4] The model used here has the further virtues of keeping the density matrix always diagonal—as it should be in a classical system and introducing the oscillatory modes via the memory inherent in a momentum variable—as actually occurs in a real fluid.



(a) (b)

FIG. 3. A process represented by the transition matrix T^C. Two particles, whose momenta, represented by the arrows add up to zero, scatter from the configuration shown in Figs. (3a) to that shown in (3b) where the final momenta again add up to zero. These particles can scatter with equal probability into any momentum values which add up to zero total momentum.

C. Local Equilibrium Solution

In this section, we describe the transport properties of the model defined in the last section. We will show that standard transport behavior of sound waves and heat waves will emerge from the local equilibrium approximation. Hence this model has some very satisfactory qualitative features. However, one should recognize that because $\mathbf{T}$ is non-Hermitian, we have not been able to prove that the local equilibrium approximation gives the correct temperature dependence for the transport coefficients very close to the critical point. In fact, we are hopeful that the local equilibrium approximation is very inaccurate near the critical point. Real fluid phase transitions show infinities in transport coefficients at the critical point; the local equilibrium approximation does not. Preliminary calculations indicate that this model gives an infinite thermal conductivity at the critical point when one employs a more accurate calculational scheme that the local equilibrium approximation.

The local equilibrium approximation uses the approximate eigenstate

$$|t\rangle = e^{-st} p_{eq}[\,|n,\mathbf{q}\rangle\delta\mu - |\epsilon,\mathbf{q}\rangle\delta\beta + |\mathbf{g},\mathbf{q}\rangle\cdot\delta\mathbf{v}], \quad (4.20)$$

where

$$\begin{aligned} |n,\mathbf{q}\rangle &= (1/\sqrt{N}) \sum_\mathbf{r} e^{i\mathbf{q}\cdot\mathbf{r}} m(\mathbf{r})|\,\rangle, \\ |\epsilon,\mathbf{q}\rangle &= (1/\sqrt{N}) \sum_\mathbf{r} e^{i\mathbf{q}\cdot\mathbf{r}} \epsilon(\mathbf{r})|\,\rangle, \\ |\mathbf{g},\mathbf{q}\rangle &= (1/\sqrt{N}) \sum_\mathbf{r} e^{i\mathbf{q}\cdot\mathbf{r}} \mathbf{g}_\mathbf{r}|\,\rangle. \end{aligned} \quad (4.21)$$

In Eq. (4.20), $\delta\mu$, $\delta\beta$, and $\delta\mathbf{v}$ represent variations in the local chemical potential, inverse temperature, and velocity. The equilibrium density matrix is taken at $\mathbf{v}=\mathbf{0}$.

In order to eliminate the simplest case first, let $\delta\mathbf{v}$ point in the x direction and $\mathbf{q}$ point in the y direction. This transverse momentum flow does not involve a $\delta\mu$ or $\delta\beta$. Then the approximate master equation becomes

$$-sp_{eq}|\mathbf{g},\mathbf{q}\rangle\cdot\delta\mathbf{v}=p_{eq}\mathbf{T}|\mathbf{g},\mathbf{q}\rangle\cdot\delta\mathbf{v}.$$

We multiply this equation on the left by $\langle g_x,\mathbf{q}|$ and find

$$-s\langle g_x,\mathbf{q}|p_{eq}|g_x,\mathbf{q}\rangle\delta v=\langle g_x,\mathbf{q}|p_{eq}\mathbf{T}|g_x,\mathbf{q}\rangle\delta v. \quad (4.22)$$

The left-hand side of Eq. (4.22) is simply the time derivative of the average momentum which appears in response to the velocity disturbance. Since g's at different sites are uncorrelated in equilibrium, the left-hand side is easily evaluable. In two dimensions

$$-s\tfrac{1}{2}(1+\langle\langle\sigma_\mathbf{r}\rangle\rangle)\delta v=-s\langle g_x,\mathbf{q}|p_{eq}|g_x,\mathbf{q}\rangle\delta v. \quad (4.23)$$

In three dimensions, there is an extra factor of $\frac{2}{3}$ on the left-hand side of Eq. (4.23). The right-hand side of Eq. (4.22) has the meaning of $\nabla^2 v$ times the viscosity η. Hence the approximate eigenvalue of $-\mathbf{T}$ is for three dimensions

$$s=3q^2\eta/(1+\langle\langle\sigma_\mathbf{r}\rangle\rangle), \quad (4.24)$$

while

$$\eta=-(1/q^2)\langle g_x,\mathbf{q}|p_{eq}\mathbf{T}|g_x,\mathbf{q}\rangle. \quad (4.25)$$

Because $\mathbf{T}^B$ drives particles in the direction of their momentum, it makes no contribution to Eq. (4.25). The contributions from $\mathbf{T}^A$ and $\mathbf{T}^C$ are

$$\eta^A=-\frac{1}{q^2}\sum_{\mathbf{r},\mathbf{r}'}\frac{w^A}{2N}\sum_{\mathbf{r}_1\mathbf{r}_2}e^{-iq(y_1-y_2)}\times\langle|(\mathbf{g}_{\mathbf{r}_1})_x(\mathbf{I}_{\mathbf{r},\mathbf{r}'}-\mathbf{1})\Delta_{\mathbf{r},\mathbf{r}'}{}^A(\mathbf{g}_{\mathbf{r}_2})_x|eq\rangle$$

$$=-\frac{1}{q^2}\sum_{\mathbf{r},\mathbf{r}'}\frac{w^A}{4N}[1-\cos q(y-y')]\times\langle|[(\mathbf{g}_\mathbf{r})_x-(\mathbf{g}_{\mathbf{r}'})_x]\Delta_{\mathbf{r},\mathbf{r}'}{}^A[(\mathbf{g}_\mathbf{r})_x-(\mathbf{g}_{\mathbf{r}'})_x]|eq\rangle.$$

For small q in two dimensions this gives

$$\eta^A=\sum_{\mathbf{r},\mathbf{r}'}\langle\langle\Delta_{\mathbf{r},\mathbf{r}'}{}^A\rangle\rangle\frac{w^A}{4N}$$

$$=w^A\langle\langle\tfrac{1}{2}(1-\sigma_\mathbf{r}\sigma_{\mathbf{r}'})\delta(u_\mathbf{r},u_{\mathbf{r}'})\rangle\rangle. \quad (4.26a)$$

The last form of writing holds when $\mathbf{r}$ and $\mathbf{r}'$ are any pair of next-nearest neighbors. In writing Eq. (4.26a), we have taken the lattice constant to be unity.

A roughly similar calculation gives

$$\eta^C=w^C\langle\langle\tfrac{1}{2}(1+\sigma_\mathbf{r})\tfrac{1}{2}(1+\sigma_{\mathbf{r}'})\rangle\rangle \quad (4.26b)$$

in two dimensions. Here $\mathbf{r}$ and $\mathbf{r}'$ are any pair of nearest neighboring sites. Hence the local equilibrium approximation correctly describes the diffusion of the transverse component of the momentum and predicts a finite shear viscosity.

Now, return to the more complex structure in Eq. (4.20) and take $\mathbf{v}$ and $\mathbf{q}$ to be parallel to the x direction. The master equation reads

$$-s|t\rangle=\mathbf{T}|t\rangle.$$

If we take matrix elements of the master equation by multiplying on the left by $\langle n,\mathbf{q}|$, $\langle\epsilon,\mathbf{q}|$, and $\langle g_x,\mathbf{q}|$, we obtain the following set of equations for small q:

$$-s\left[\left(\frac{\partial n}{\partial\mu}\right)_\beta\delta\mu-\left(\frac{\partial n}{\partial\beta}\right)_\mu\delta\beta\right]=-q^2[\lambda_{nn}\delta\mu-\lambda_{n\epsilon}\delta\beta]-i\mathbf{q}\cdot\rho\delta\mathbf{v}, \quad (4.27a)$$

$$-s\left[-\left(\frac{\partial n}{\partial\beta}\right)_\mu\delta\mu+\left(\frac{\partial\epsilon}{\partial\beta}\right)_\mu\delta\beta\right]=-q^2[-\lambda_{\epsilon n}\delta\mu+\lambda_{\epsilon\epsilon}\delta\beta]-i\mathbf{q}\cdot\rho^\epsilon\delta\mathbf{v}. \quad (4.27b)$$

Finally, in three dimensions, the time derivative of the momentum density is

$$-s\left[\frac{2}{3}\frac{(1+\langle\langle\sigma_\mathbf{r}\rangle\rangle)}{2}\right]\delta\mathbf{v}=-\mathbf{iq}[\rho\delta\mu+\rho^\epsilon\delta\beta]-q^2[\zeta+\tfrac{4}{3}\eta]\delta\mathbf{v}. \quad (4.27c)$$

In two dimensions, the factor $\frac{2}{3}$ on the left-hand side of Eq. (4.27c) is replaced by unity.

These equations look quite complex, but they have a simple physical interpretation. The left-hand sides are the time derivatives of the number density, energy density, and momentum density evaluated for local equilibrium. The thermodynamic derivatives are evaluated in the lattice gas. The only difference from the usual case is that our μ is the usual μ/kT. The derivative

$$\left(\frac{\partial n}{\partial\mu}\right)_\beta=\sum_{\mathbf{r},\mathbf{r}'}\frac{1}{N}\langle\langle[\sigma_\mathbf{r}-\langle\langle\sigma_\mathbf{r}\rangle\rangle][\sigma_{\mathbf{r}'}-\langle\langle\sigma_{\mathbf{r}'}\rangle\rangle]\rangle\rangle \quad (4.28)$$

describes the infinite compressibility of the usual lattice gas at the critical point. Also $(\partial\epsilon/\partial\beta)_\mu$ is proportional to C_v. The terms involving λ's are the transport coefficients. For example,

$$\lambda_{\epsilon\epsilon}=-(1/q^2)\langle\epsilon,\mathbf{q}|p_{eq}\mathbf{T}|\epsilon,\mathbf{q}\rangle \quad (4.29)$$

is essentially the thermal conductivity. Because the translation invariance has been lost there is a particle diffusion coefficient λ_{nn} and a thermal diffusion coefficient $\lambda_{n\epsilon}$ as in a two-component gas. The approximation also includes an Onsager relation $\lambda_{n\epsilon}=\lambda_{\epsilon n}$.

The standard longitudinal viscosity which appears in Eq. (4.27c) is

$$\zeta+\tfrac{4}{3}\eta=-(1/q^2)\langle g_x,\mathbf{q}|p_{eq}\mathbf{T}|g_x,\mathbf{q}\rangle, \quad (4.30)$$

where q points in the x direction. Finally Eq. (4.27c) contains an analog of the gradient of the pressure as the first square bracket on its right-hand side.

Sound waves arise from Eq. (4.27) because of the drift currents $\rho\delta\mathbf{v}$ and $\rho^\epsilon\delta\mathbf{v}$ in Eqs. (4.27a) and (4.27b) and because of the "pressure gradient"

$$-i\mathbf{q}[\rho\delta\mu+\rho^\epsilon\delta\beta]$$

in Eq. (4.27c). These terms appear as

$$\begin{aligned}-i\mathbf{q}\rho&=\langle\mathbf{g},\mathbf{q}|\mathbf{T}p_{eq}|n,\mathbf{q}\rangle\\&=\langle n,\mathbf{q}|\mathbf{T}p_{eq}|\mathbf{g},\mathbf{q}\rangle,\end{aligned}\tag{4.31a}$$

$$\begin{aligned}-i\mathbf{q}\rho^\epsilon&=-\langle\mathbf{g},\mathbf{q}|\mathbf{T}p_{eq}|\epsilon,\mathbf{q}\rangle\\&=-\langle\epsilon,\mathbf{q}|\mathbf{T}p_{eq}|\mathbf{g},\mathbf{q}\rangle.\end{aligned}\tag{4.31b}$$

Notice that ρ appears in two places: The drift current is proportional to $\rho\mathbf{v}$ and the "pressure gradient" contains $\rho\delta\mu$. These two ρ's are identical because there is a kind of "Onsager relation" between the off-diagonal matrix elements of $\mathbf{T}$. In the usual transport theory these relations appear as the statement that the particle current is $n\mathbf{v}$ while the pressure obeys $(\partial p/\partial\mu)_T=n$.

We can evaluate ρ most conveniently by employing the second of Eqs. (4.31). The only part of $\mathbf{T}$ which contributes to ρ is the non-Hermitian term $\mathbf{T}^B$. We find when q points in the x direction

$$\begin{aligned}-iq\rho&=\langle n,\mathbf{q}|\mathbf{T}^Bp_{eq}|g_x,\mathbf{q}\rangle\\&=\sum_{\mathbf{r},\mathbf{r}'}\frac{w^B}{N}\sum_{\mathbf{r}_1,\mathbf{r}_2}e^{-i\mathbf{q}\cdot(\mathbf{r}_1-\mathbf{r}_2)}\langle|\sigma_{\mathbf{r}_1}(\mathbf{I}_{\mathbf{r},\mathbf{r}'}-\mathbf{1})\Delta_{\mathbf{r},\mathbf{r}'}{}^B(\mathbf{g}_{\mathbf{r}_2})|eq\rangle\\&=-\frac{2w^B}{N}\sum_{\mathbf{r},\mathbf{r}_2,\mathbf{r}_1,\mathbf{r}_2}[e^{-i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}_2)}-e^{-i\mathbf{q}\cdot(\mathbf{r}'-\mathbf{r}_2)}]\\&\qquad\times\langle|\Delta_{\mathbf{r},\mathbf{r}'}{}^B(\mathbf{g}_{\mathbf{r}_2})_x|eq\rangle.\end{aligned}$$

Since $\Delta_{\mathbf{r},\mathbf{r}'}{}^B$ only depends upon the value of $\mathbf{g}_{\mathbf{r}_1}$ at $\mathbf{r}_2=\mathbf{r}$, only the term with $\mathbf{r}_2=\mathbf{r}$ contributes to the sum. Thus, for small q,

$$-iq\rho=-\frac{2w^B}{N}\sum_{\mathbf{r},\mathbf{r}'}i\mathbf{q}\cdot(\mathbf{r}'-\mathbf{r})\langle|\Delta_{\mathbf{r},\mathbf{r}'}{}^B(\mathbf{g}_{\mathbf{r}})_x|eq\rangle$$

or

$$\rho=\frac{2w^B}{N}\sum_{\mathbf{r},\mathbf{r}'}(x'-x)\langle|\Delta_{\mathbf{r},\mathbf{r}'}{}^B(\mathbf{g}_{\mathbf{r}})_x|eq\rangle.\tag{4.32}$$

Notice that $\Delta_{\mathbf{r},\mathbf{r}'}{}^B$ sends a particle from $\mathbf{r}$ to $\mathbf{r}'$ in the direction of $\mathbf{g}_{\mathbf{r}}$. Then, inside the sum

$$(x'-x)=|x'-x|(\mathbf{g}_{\mathbf{r}})_x.$$

Consequently,

$$\rho=\frac{2w^B}{N}\sum_{\mathbf{r},\mathbf{r}'}|x'-x|\langle|\Delta_{\mathbf{r},\mathbf{r}'}{}^B[(\mathbf{g}_{\mathbf{r}})_x]^2|eq\rangle.\tag{4.33}$$

Equation (4.33) indicates that ρ is positive and finite.

Direct calculations of matrix elements show that all quantities in Eqs. (4.27) are finite everywhere save the thermodynamic derivatives $(\partial n/\partial\beta)_\mu$, $(\partial n/\partial\mu)_\beta$, $(\partial\epsilon/\partial\beta)_\mu$ which may diverge at the critical point. As an example, a calculation of λ_{nn} is given in an appendix.

Without further ado, we may conclude that all transport coefficients are finite in this local equilibrium approximation. However, the approximation is not variational because $\mathbf{T}$ is not Hermitian. Hence we really know nothing about the exact transport coefficients.

The approximate eigenvalues of s in the local equilibrium approximation are determined by the condition that the 3×3 matrix of Eqs. (4.27) have zero determinant. For small q this condition gives: first, a diffusion mode with

$$s=\frac{\lambda_{nn}(\rho^\epsilon)^2+2\lambda_{n\epsilon}\rho\rho^\epsilon+\lambda_{\epsilon\epsilon}\rho^2}{(\partial n/\partial\mu)_\beta(\rho^\epsilon)^2+2(\partial n/\partial\beta)_\mu\rho^\epsilon\rho+(\partial\epsilon/\partial\beta)_\mu\rho^2}q^2.\tag{4.34}$$

Near the critical point, the term in $(\partial n/\partial\mu)_\beta$ dominates the denominator. Hence according to this model the thermal diffusivity goes to zero as the inverse compressibility.

The other modes are sound waves with

$$s^2=-c^2q^2\tag{4.35}$$

and sound velocity squared

$$c^2=\frac{\rho}{\langle\langle[(g_{\mathbf{r}})_x]^2\rangle\rangle}[\rho(\partial\mu/\partial n)_s+\rho^\epsilon(\partial\beta/\partial n)_s],\tag{4.36}$$

where fixed s means

$$\rho dn=\rho^\epsilon d\epsilon$$

or

$$\begin{aligned}&\rho[(\partial n/\partial\mu)_\beta d\mu-(\partial n/\partial\beta)_\mu d\beta]\\&\qquad=\rho^\epsilon[-(\partial n/\partial\beta)_\mu d\mu+(\partial\epsilon/\partial\beta)_\mu d\beta].\end{aligned}\tag{4.37}$$

Thus c^2 goes to zero as $T\to T_c$.

The modes are then qualitatively correct, but further work is necessary to establish whether or not the transport coefficients are actually finite.

APPENDIX: CALCULATION OF λ_{nn} IN TWO DIMENSIONS

The expression for λ_{nn} is

$$\lambda_{nn}=-(1/q^2)\langle n,\mathbf{q}|p_{eq}\mathbf{T}|n,\mathbf{q}\rangle.\tag{A1}$$

Since the process described by the transition matrix $\mathbf{T}^c$ involves no interchange of particles, $\mathbf{T}^c$ does not contribute to λ_{nn}. The contribution to λ_{nn} from the $\mathbf{T}^A$ term is λ_{mm} which is given in Eq. (3.14a) and is obviously finite. Consequently, we concentrate on the contribution due to $\mathbf{T}^B$

$$\begin{aligned}\lambda_{nn}{}^B&=-(1/q^2)\langle n,\mathbf{q}|\mathbf{T}^Bp_{eq}|n,\mathbf{q}\rangle\\&=-\frac{1}{q^2}\frac{w^B}{N}\sum_{\mathbf{r},\mathbf{r}',\mathbf{r}_1,\mathbf{r}_2}e^{-i\mathbf{q}\cdot(\mathbf{r}_1-\mathbf{r}_2)}\\&\qquad\times\langle|\sigma_{\mathbf{r}_1}(\mathbf{I}_{\mathbf{r},\mathbf{r}'}-\mathbf{1})\Delta_{\mathbf{r},\mathbf{r}'}{}^B\sigma_{\mathbf{r}_2}|eq\rangle.\end{aligned}\tag{A2}$$

If the equilibrium state has $\mathbf{v}=\mathbf{0}$, we can easily average over the directions of all the momenta. We represent the result of this averaging by the replacement

$$\Delta_{\mathbf{r},\mathbf{r}'}{}^{B} \rightarrow \tfrac{1}{2}(1+\sigma_{\mathbf{r}})\tfrac{1}{2}(1-\sigma_{\mathbf{r}'})\bar{\Delta}_{\mathbf{r},\mathbf{r}'}{}^{B}/[2d(d-1)], \quad \text{(A3)}$$

where d is the dimensionality of the lattice. The factor $2d(d-1)$ gives the number of different $\mathbf{g}_{\mathbf{r}}$'s which can contribute. The factor $\bar{\Delta}_{\mathbf{r},\mathbf{r}'}{}^{B}$ is

$$\bar{\Delta}_{\mathbf{r},\mathbf{r}'}{}^{B}=\delta(u_{\mathbf{r}},u_{\mathbf{r}'})\tfrac{1}{2}(1-\sigma_{\mathbf{r}}\sigma_{\mathbf{r}'})\theta_{\mathbf{r},\mathbf{r}'},$$

when $\mathbf{r}-\mathbf{r}'$ is parallel to a nearest-neighbor direction and is zero otherwise. Therefore, the matrix element in Eq. (A2) is

$$\mathbf{M}_{\mathbf{r},\mathbf{r}'}=\langle\,|\sigma_{\mathbf{r}_1}(\mathbf{I}_{\mathbf{r},\mathbf{r}'}-\mathbf{1})\tfrac{1}{2}(1+\sigma_{\mathbf{r}})\tfrac{1}{2}(1+\sigma_{\mathbf{r}'})\bar{\Delta}_{\mathbf{r},\mathbf{r}'}{}^{B}\sigma_{\mathbf{r}_2}|eq\rangle \times 1/[2d(d-1)]. \quad \text{(A4)}$$

Because of the sum over $\mathbf{r}$ and $\mathbf{r}'$ we can replace $\mathbf{M}_{\mathbf{r},\mathbf{r}'}$ inside the sum by

$$\mathbf{M}_{\mathbf{r},\mathbf{r}'} \rightarrow \tfrac{1}{2}(\mathbf{M}_{\mathbf{r},\mathbf{r}'}+\mathbf{M}_{\mathbf{r}',\mathbf{r}}) =\langle\,|\sigma_{\mathbf{r}_1}(\mathbf{I}_{\mathbf{r},\mathbf{r}'}-\mathbf{1})\bar{\Delta}_{\mathbf{r},\mathbf{r}'}{}^{B}\sigma_{\mathbf{r}_2}|eq\rangle/[4d(d-1)], \quad \text{(A5)}$$

but $\mathbf{I}_{\mathbf{r},\mathbf{r}'}$ commutes with $\bar{\Delta}_{\mathbf{r},\mathbf{r}'}{}^{B}$. Therefore we can insert a factor $\frac{1}{2}(\mathbf{1}-\mathbf{I}_{\mathbf{r},\mathbf{r}'})$ just to the right of $\bar{\Delta}_{\mathbf{r},\mathbf{r}'}{}^{B}$ without changing the matrix element at all, since this factor is just a projection operator. When this replacement is made and $\mathbf{M}_{\mathbf{r},\mathbf{r}'}$ is reinserted in Eq. (A2), this equation becomes

$$\lambda_{nn}{}^{B}=\frac{1}{q^2}\frac{w^{B}}{4d(d-1)N}\sum_{\mathbf{r}_1,\mathbf{r}_2}\sum_{\mathbf{r},\mathbf{r}'}e^{-i\mathbf{q}\cdot(\mathbf{r}_1-\mathbf{r}_2)} \times\langle\,|\sigma_{\mathbf{r}_1}\tfrac{1}{2}(1-\mathbf{I}_{\mathbf{r},\mathbf{r}'})\bar{\Delta}_{\mathbf{r},\mathbf{r}'}{}^{B}\tfrac{1}{2}(1-\mathbf{I}_{\mathbf{r},\mathbf{r}'})\sigma_{\mathbf{r}_2}|eq\rangle. \quad \text{(A6)}$$

Now, the only terms which can possibly contribute to the sum over $\mathbf{r}_1$ and $\mathbf{r}_2$ are those with $\mathbf{r}_1=\mathbf{r}$ and $\mathbf{r}'$ and also $\mathbf{r}_2=\mathbf{r}$ and $\mathbf{r}'$. Otherwise the projection operators give zero. With this restriction, Eq. (A6) becomes

$$\lambda_{nn}{}^{B}=\frac{w^{B}}{4d(d-1)N}\sum_{\mathbf{r},\mathbf{r}'}\frac{2-2\cos\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')}{q^2}\langle\langle\bar{\Delta}_{\mathbf{r},\mathbf{r}'}{}^{B}\rangle\rangle. \quad \text{(A7)}$$

For small q this reduces to

$$\lambda_{nn}{}^{B}=\frac{w^{B}}{4d^2(d-1)N}\sum_{\mathbf{r},\mathbf{r}'}(\mathbf{r}-\mathbf{r}')^2\langle\langle\bar{\Delta}_{\mathbf{r},\mathbf{r}'}{}^{B}\rangle\rangle. \quad \text{(A8)}$$

Since $\mathbf{r}-\mathbf{r}'$ must be parallel to a next-nearest-neighbor axis

$$\lambda_{nn}{}^{B}=\frac{w^{B}}{d}\sum_{n=1}^{\infty}n^2\langle\langle\bar{\Delta}_{\mathbf{r},\mathbf{r}}{}^{B}{}_{+\mathbf{e}n}\rangle\rangle, \quad \text{(A9)}$$

where $\mathbf{e}$ is any vector which takes you from a particle to its next-nearest neighbor. More explicitly

$$\lambda_{nn}{}^{B}=\frac{w^{B}}{d}\sum_{n=1}^{\infty}n^2 \times\langle\langle\delta(u_{\mathbf{r}},u_{\mathbf{r}}+n\mathbf{e})\tfrac{1}{2}(1-\sigma_{\mathbf{r}}\sigma_{\mathbf{r}+n\mathbf{e}})\theta_{\mathbf{r}',\mathbf{r}+n\mathbf{e}}\rangle\rangle. \quad \text{(A10)}$$

Since θ requires that there be no holes which lie between $\mathbf{r}$ and $\mathbf{r}+n\mathbf{e}$, the sum over n gains exponentially small contributions from large n. Hence the local equilibrium approximation transport coefficient is finite.