PHYSICAL REVIEW E VOLUME 52, NUMBER 1 JULY 1995

Correlations and renormalization in lattice gases

Bruce M. Boghosian*
Center for Computational Science, Boston University, 3 Cummington Street, Boston, Massachusetts 02215

Washington Taylor†
Center for Theoretical Physics, Laboratory for Nuclear Science and Department of Physics,
Massachusetts Institute of Technology, Cambridge, Massachusetts 02139

(Received 22 April 1994; revised manuscript received 9 February 1995)

An exact kinetic theory is formulated for lattice gases. This kinetic theory makes possible the calculation of corrections to the usual combined Boltzmann and Chapman-Enskog analysis of lattice gases due to the buildup of correlations. Cluster expansion methods are used to show that renormalized transport coefficients for lattice gases satisfying semidetailed balance can be calculated perturbatively by summing terms in an infinite series. A diagrammatic notation for the terms in this series is given, in analogy with the diagrammatic expansions of continuum kinetic theory and quantum field theory. A closed-form expression for the coefficients associated with the vertices of these diagrams is given. This method is applied to several standard lattice gases, and the results are shown to correctly predict observed deviations from the Boltzmann analysis.

PACS number(s): 05.20.Dd, 05.50.+q, 64.60.Cn

I. INTRODUCTION

Lattice gases are a class of dynamical systems in which particles move on a lattice in discrete time steps. In much the same way that the Ising model and other similar lattice spin models provide simple examples of equilibrium statistical mechanical systems, lattice gases capture many features of nonequilibrium statistical mechanical systems such as fluids.

Most work on lattice gases has been done in a framework where the Boltzmann assumption is made, neglecting all correlations between the particles moving on the lattice. In this paper we give a complete description of a theory of lattice gases in which the effects of all correlations are included. For a wide variety of lattice gases, the effect of these correlations is only to correct or *renormalize* the hydrodynamic transport coefficients, and we show how to compute this correction. For some lattice gases, the resulting renormalization can change parameters in the theory by substantial amounts, so that in any situation where lattice gases are used to make precise quantitative predictions, the effects of correlations should be considered and the magnitude of the resulting correction to the usual analysis should be estimated.

A. Background

In 1986, it was shown [1] that lattice gases could be used to simulate two-dimensional Navier-Stokes flow. Since then, lattice gases have been developed to describe a wide variety of physical systems. Examples are three-dimensional Navier-Stokes flow [2], magnetohydrodynamics [3], immiscible fluids with a surface tension interface [4,5], convection [6], two-phase liquid-gas flow [7], Burgers's equation [8], and reaction-diffusion equations [9]. For a summary of recent works on the subject, see the proceedings edited by Doolen [10,11], by Monaco [12], by Manneville *et al.* [13], by Alves [14], and by Boon and Lebowitz [15].

Why should we expect the bulk behavior of particles moving and colliding on a lattice to be that of a fluid? In nature, we observe that many different fluids, with drastically differing intermolecular force laws, satisfy the Navier-Stokes equations to a reasonable degree of approximation. In spite of all the differences between the intermolecular collisions of, say, water and molasses, both types of collisions conserve mass and momentum; ultimately the existence of these conserved quantities gives rise to fluidlike behavior at the macroscopic level. (Conservation of mass and momentum is sufficient to get the correct behavior in the incompressible regime. To get correct *compressible* behavior, it is necessary to conserve energy as well.) A lattice-gas model can be thought of as an attempt to find the simplest possible dynamical system with these conservation laws.

The idea that macroscopic properties of a physical system should be independent of the microscopic definition of the system is also a familiar concept in equilibrium statistical mechanics and in quantum field theory. In such theories, the effect of looking at the physics of the system at larger and larger scales is mathematically described by the renormalization group flow of the system [16]. Generally, as the scale of the physics of interest becomes extremely large compared to the scale at which the system is defined, one finds that the renormalization-group flow takes the system towards certain fixed points, which describe entire universality classes of theories with identical macroscopic behavior. The emergence of similar hydro-

---

*Electronic address: bruceb@bu.edu
†Electronic address: wati@mit.edu

1063-651X/95/52(1)/510(45)/$06.00

dynamic equations in a variety of systems with different microscopic dynamics is an equivalent phenomenon in nonequilibrium statistical mechanics.

Of course, there are some properties of fluids in which the details of the microscopic collisions manifest themselves at the macroscopic level. The most obvious such properties are the transport coefficients. While water and molasses both satisfy the Navier-Stokes equations, they do so with very different viscosities. Long-time tails in velocity autocorrelation functions are also well known to be sensitive to the microscopic dynamics.

The central problem in the theoretical analysis of a lattice gas is thus the determination of the macroscopic hydrodynamic equations obeyed by the conserved quantities of the system, with the transport coefficients expressed as functions of those conserved quantities. This is the classical problem of kinetic theory. The methods needed to perform this analysis for continuum fluids have been well developed over the past century [17]. Two key approximations are used in the course of such analyses.

(i) The *Boltzmann molecular chaos approximation* (or *Stosszahlansatz*) neglects correlations between molecules entering a collision. This makes it possible to obtain a single closed equation, called the *Boltzmann equation*, for the single-particle distribution function.

(ii) The *Chapman-Enskog analysis* is an asymptotic expansion in Knudsen number that yields closed hydrodynamic equations for the conserved quantities. (The Knudsen number is the ratio of mean free path to the macroscopic scale length.)

During the 1960s and 1970s, much work centered on the removal of the first of these two approximations for continuum fluids [18,19] and for Lorentz gases [20]. It was found that the buildup of correlations between the molecules of a fluid could seriously alter, or *renormalize*, the transport coefficients predicted by the Boltzmann theory. Expressions for these corrections were derived in terms of diagrammatic sums. The propagators in these diagrams can be thought of as propagating correlated quantities; the vertices describe collisions in which correlated quantities interact. Thus an event in which two particles emerge from a collision (and thereby acquire a correlation), move about in a background of uncorrelated particles, and later recollide, can be thought of as a one-loop correction to the Boltzmann approximation. Further refinements can be obtained by including more intricate diagrams—with multiple loops, nested loops, etc.—to account for the interaction of the correlated quantities with the background. Standard field-theoretic techniques can then be used to approximate these diagrammatic sums.

As part of the recent flurry of interest in lattice gases, much of classical kinetic theory has been extended to lattice gases. In particular, the derivation of Boltzmann equations for lattice gases and the application of the Chapman-Enskog theory has been well understood for several years now thanks to the works of a number of authors [21,2]. While these works have generally capitalized on the similarities between lattice gases and continuum fluids, they have also pointed to some very important differences between the two.

The most important of these differences has to do with the assumptions leading up to the derivation of the Boltzmann equation. Though the assumption of molecular chaos is made in either case, the analysis of continuum fluids generally proceeds under the additional assumption that the fluid is *dilute*, that is, that collisions involving more than two molecules can be ignored. For lattice gases, on the other hand, it is essential that tertiary and higher collision events be treated properly. For example, tertiary collisions are essential to the success of the Frisch-Hasslacher-Pomeau (FHP-I) lattice gas because they break an unphysical (spurious) conserved quantity [1]. In addition, the inclusion of higher-order collision events has been shown to decrease the viscosity of fluid lattice gases, thereby making possible higher Reynolds number simulations [21].

Thus collision operators for lattice gases routinely include terms for tertiary and higher-order collisions. While this is really only a minor nuisance in the Boltzmann and Chapman-Enskog analyses, it introduces a significant complication to the exact kinetic theory. The kinetic theory of dilute fluids needs to consider only those vertices for which two or fewer correlated quantities enter and exit. Lattice-gas kinetic theory, on the other hand, must additionally treat vertices involving three or more entering and/or exiting correlated quantities. The number of correlated quantities that can enter and/or exit a vertex is limited only by the number of lattice vectors at a site. This gives rise to a much richer diagrammatic series than is the case for a dilute continuum fluid.

Another difference between continuum fluids and lattice gases, which gives the kinetic theories for these types of systems very different flavors, is the simple fact that continuum fluids are defined on continuous spaces while lattice gases are defined on discrete spaces. The consequence of this difference is that while corrections due to correlations in continuum fluids are expressed in terms of complicated integral expressions, the corrections in lattice gases are given by combinatorial sums over countable sets of graphs. Thus the problem of calculating exact transport coefficients in a lattice gas becomes essentially a combinatorial, rather than an analytic, problem.

For some lattice gases the corrections to the transport coefficients arise from diagrams that extend spatially and temporally over only a short distance on the lattice, i.e., a distance that goes to zero in the scaling limit. The resulting rapid convergence of the formulas for transport coefficients makes these lattice-gas systems extremely attractive both as models with which to study complicated properties of related physical systems in the continuum and as pedagogical tools with which to describe the essential features of a complete kinetic theory without the complications associated with continuum systems.

B. Results presented in this paper

In this paper, we give a complete formulation of an exact kinetic theory of lattice gases. We prove that for a wide class of lattice gases, the effects of correlations can be completely described by a renormalization of the transport coefficients. Furthermore, we give explicit formulas for the renormalized transport coefficients in terms of a sum over an infinite set of diagrams. We describe the renormalization calculation in detail for several specific lattice gases and discuss a variety of methods for approximating the complete diagrammatic sum.

We begin with a review of the Boltzmann and Chapman-Enskog theories. We derive formulas for the hydrodynamic equations of a general class of lattice gases. We then apply this general formalism to four example lattice gases, three of which are familiar from the literature; for these three the Chapman-Enskog analysis has been previously carried out using more specific methods. Our intent in this part of the paper is to describe the general formalism in a concise fashion and to illustrate its application to simple model problems, thereby providing a context for our subsequent development of the diagrammatic renormalization theory. Our presentation of the combined Boltzmann–Chapman-Enskog analysis contains the following features and results.

(i) The formulas we derive for the hydrodynamic equations and the transport coefficients of semidetailed balance (SDB) lattice gases have, to our knowledge, never before been written down in this generality.

(ii) Our results are presented in a mathematical framework that is interesting in its own right. We introduce a family of metrics on the space of local Gibbsian equilibria and show that the transport coefficients can be expressed quite naturally in terms of these metrics and their associated Christoffel symbols.

(iii) For the special case of lattice fluids on a regular lattice with single-speed particles, we derive an expression for the viscosity that agrees with that of Hénon and yields an alternative and compact form for the quantity that he calls λ in his paper on the subject [22].

Next we present the exact kinetic theory for lattice gases. We introduce the general theory with a specific example of how correlations renormalize transport coefficients. The main features of the general theory are as follows.

(i) We give a simple expression for the renormalized transport coefficients of any lattice gas obeying SDB at lowest order in the Chapman-Enskog expansion parameter. The transport coefficients are given in terms of a sum over an infinite set of terms, each associated with a diagram describing the propagation and interaction of a set of correlations.

(ii) We show that the correction associated with each diagram can be decomposed into a product of elementary factors associated with the vertices in the diagram; these factors describe the interactions of correlated quantities at a single lattice site. Furthermore, we give a closed-form expression for these vertex coefficients.

(iii) In this paper we analyze lattice gases that either obey semidetailed balance or violate it at subleading order in the expansion parameter ϵ; we always assume that the equilibrium is at most $O(\epsilon)$ away from a Gibbsian distribution. We show that when a lattice gas violates semidetailed balance at higher order in the expansion parameter, the effects of correlations can give rise to renormalized source terms in the hydrodynamic equations in addition to the usual renormalization of transport coefficients. We describe these renormalized source terms in terms of the same types of diagrams used to describe the renormalized transport coefficients.

(iv) We formulate the theory in terms of connected correlation functions. A similar expansion in terms of products of fluctuations was previously used to derive the ring kinetic theory for lattice gases [23,24] and for lattice Lorentz gases [25]. The use of the connected correlation functions significantly simplifies the complete diagrammatic expansion for the kinetic theory.

(v) We describe a variety of approximations that can be made to simplify the numerical computation of the renormalized transport coefficients. The simplest of these approximations is the ring approximation, in which correlations between more than two particles are neglected. Thus we find that the ring approximation results [23] are described in our theory by restricting the diagrammatic sum to the simple set of ring diagrams.

(vi) Most previous work on the kinetic ring theory of lattice gases has used the Green-Kubo formalism to obtain the series for the transport coefficients. In this paper, we use the Chapman-Enskog theory instead. In this way, we get the Boltzmann approximation at zeroth order. All higher-order terms in our series are thus corrections to the Boltzmann approximation. In the Green-Kubo theory, by contrast, it is necessary to sum an infinite number of terms (albeit simply a geometric series) just to get the Boltzmann approximation.

(vii) We work out the diagrammatic expansion in detail for four model lattice gases and we compare some of these results to lattice-gas simulations.

(viii) For one of these model problems—a lattice gas for Burgers's equation [8]—we use the diagrammatic formalism to show that the Boltzmann approximation is exact. This result has been previously obtained by other means [26]; we show that the methods introduced here significantly simplify this proof.

C. Organization of this paper

Section II begins with a review of lattice-gas theory and establishes notation that is used throughout the rest of the paper. Section III then reviews the Boltzmann and Chapman-Enskog analyses and introduces a mathematical formalism with which the results for the transport coefficients can be expressed in a simple form. Section IV contains examples in which we work out the details of this formalism for four model lattice gases.

Section V gives an example of how correlations correct the lattice-gas equations of motion. The simple calculation contained in this section serves as an introduction to the more abstract approach of Sec. VI in which we formulate the complete lattice gas kinetic theory, prove that the exact transport coefficients are expressible as the sum of a diagrammatic series, and give a closed-form expression for the vertex coefficients. Section VII contains detailed calculations of the vertex coefficients for the four model lattice gases described in Sec. IV and presents the results for the transport coefficients of these lattice gases as formal diagrammatic series. For the Burgers equation lattice gas we show that the diagrammatic series of corrections to the Boltzmann approximation vanishes, in agreement with previous work [26].

Since, with the exception of the Burgers equation example, these diagrammatic series are difficult to sum without resorting to numerical methods, Sec. VI includes a discussion of approximation schemes, including summations for short times, summations over one-loop diagrams (ring approximation), and summations over subsets of diagrams that correspond to truncations of the Bogoliubov-Born-Green-Kirkwood-Yvon (BBGKY) hierarchy. In Sec. VIII we apply several of these approximation schemes to one of the model problems (the 1D3P lattice gas) and we present comparisons to computer experiment showing that our theory correctly predicts observed deviations from the Boltzmann theory to within measurable accuracy. In this section, we also develop further approximation techniques valid for general lattice gases.

II. REVIEW OF LATTICE-GAS THEORY

A. Definitions and notation

A lattice gas is generally described by a state space and a time-development rule. The state space is defined by associating n bits with each point on a lattice L. (Bits are variables taking values in $\{0,1\}$.) We define the set of bits at a general lattice site to be B, so that $|B|=n$. We denote the total number of bits on the lattice by $N=n|L|$. For each value of the discrete time parameter t, we write the values of the bits as $n^i(\mathbf{x},t)$, where $\mathbf{x}\in L$ and $i\in B$. As noted in Sec. I, these bits can be thought of as a set of occupation numbers for individual *particle* states.

We define the set S of possible states of the bits at a general lattice point at a fixed value of t to be

$$S=\{s\colon s\subseteq B\}\ ,$$

where a state s is associated with the set of bits taking the value 1. We write the value of bit i in state s as

$$s^i=\begin{cases}1 & \text{if } i\in s\\ 0 & \text{otherwise}\ .\end{cases}$$

Note that $|S|=2^n$.

We shall often want to refer to the $N=n|L|$ bits of the lattice in a uniform fashion, so we introduce an enumeration of these N bits, given by a one-to-one correspondence between the sets $\mathcal{B}=\{1,2,\ldots,N\}$ and $B\times L=\{(i,\mathbf{x})\colon i\in B,\ \mathbf{x}\in L\}$. In this notation, a single bit of the lattice gas is written as n^a, $a\in\mathcal{B}$. To relate this notation to the more explicit $(i,\mathbf{x})$ notation, we express the above one-to-one correspondence by writing a and $(i,\mathbf{x})$ as functions of one another, so that

$$n^a(t)=n^{i(a)}(\mathbf{x}(a),t)$$

and

$$n^i(\mathbf{x},t)=n^{a(i,\mathbf{x})}(t)\ .$$

We shall use both notations interchangeably throughout this paper.

B. Microscopic dynamical equation

For each value of $i\in\{1,\ldots,n\}$ there is a lattice vector $\mathbf{c}^i$ such that $\mathbf{x}+\mathbf{c}^i\in L$ for every $\mathbf{x}\in L$. The evolution of a lattice gas for one time step can be divided into two substeps: (i) a *collision* substep in which the n bits at each site may alter their values to model a local *interaction* between the particles that they represent and (ii) a *propagation* substep in which the new value of bit i at site $\mathbf{x}$ moves to that of bit i at site $\mathbf{x}+\mathbf{c}^i$.

We desire an equation for $n^i(\mathbf{x},t+\Delta t)$ in terms of $n^i(\mathbf{x},t)$, where Δt denotes the time step. Suppose, for a moment, that the particles simply propagated without colliding. Then the dynamics would be described by

$$n^i(\mathbf{x}+\mathbf{c}^i,t+\Delta t)=n^i(\mathbf{x},t)\ .$$

The addition of collisions introduces a *collision operator* on the right-hand side of the above equation. That is, we have

$$n^i(\mathbf{x}+\mathbf{c}^i,t+\Delta t)=n^i(\mathbf{x},t)+\omega^i(n^*(\mathbf{x},t))\ , \tag{1}$$

where the collision operator ω^i describes the change in bit i due to collisions. Note that the form $f(z^*)$ is used to indicate dependency of a function f on a quantity z^i for all possible values of the index (in this case i) that has been replaced by the asterisk. For instance, $\omega^i(n^*(\mathbf{x},t))$ is shorthand for $\omega^i(n^1(\mathbf{x},t),n^2(\mathbf{x},t),\ldots,n^n(\mathbf{x},t))$.

C. Collision operator

The collision process at a fixed lattice site and time step can be fully specified by a $2^n\times 2^n$ Boolean *transition matrix* a, whose element $a(s\to s')$ is unity if and only if the particles in state s collide to yield particles in state s'. Since each incoming state gives rise to exactly one outgoing state,

$$\sum_{s'}a(s\to s')=1\ . \tag{2}$$

Stochastic lattice gases deserve special mention at this point. They also have $a(s\to s')$ equal to unity for exactly one value of s' for each value of s, but that value of s' may differ from site to site and from time step to time step for a fixed value of s. For example, we might have $a(s\to s_1)=r$, $a(s\to s_2)=1-r$, and $a(s\to s')=0$ for $s'\neq s_1,s_2$, where r is a random bit that is sampled at each site at each time step with some specified mean $R=\langle r\rangle$. This would effectively mean that the outcome of a collision for incoming state s is state s_1 with probability R and state s_2 with probability $1-R$. Note that Eq. (2) is still always satisfied.

If we define the Kronecker delta function of two bits

$$\delta(x,y)=\begin{cases}1 & \text{if } x=y\\ 0 & \text{otherwise}\end{cases}$$
$$=1-x-y+2xy\ , \tag{3}$$

then the product

$$\prod_{j=1}^{n}\delta(n^j,s^j)$$

is unity at a given site if and only if that site is in state s. Since the collision operator ω^i is nothing more than the total change in bit i due to collision, it can be expressed in terms of the transition matrix as

$$\omega^i(n^*)=\sum_{s,s'} a(s\to s')(s'^{\,i}-s^i)\prod_{j=1}^{n}\delta(n^j,s^j) \ . \tag{4}$$

D. Conserved quantities

Another distinguishing feature of lattice gases is the presence of some number of additive conserved quantities that are linear in the bit values. For example, in some lattice gases, the total number of particles is a conserved quantity; it is clearly conserved by the propagation phase of the time step and we can choose collision rules that conserve particle number as well.

Let us assume that we have a lattice gas with n_c of conserved quantities. We assume that all conserved quantities are linear in the configuration bit values, so we can write the value of the μth conserved quantity at site $\mathbf{x}$ and at time t in the form

$$q^{\mu}(\mathbf{x},t)=q_i^{\mu}n^i(\mathbf{x},t) \quad \text{for } \mu=1,\dots,n_c \ , \tag{5}$$

where the coefficients q_i^{μ} satisfy

$$0=q_i^{\mu}\omega^i(n^*) \quad \text{for } \mu=1,\dots,n_c \ . \tag{6}$$

It is important to note that the q_i^{μ} are constant coefficients, independent of spatial position. Throughout this paper we adopt the modified Einstein summation convention that if the same index appears in at least one contravariant position and at least one covariant position in every term where it appears at all (on either side of the equation), then it is to be summed over its entire range of values. Sometimes summations are indicated explicitly, particularly when the range of summation is not clear from the context.

From Eq. (6) it follows that

$$\begin{aligned}\sum_{\mathbf{x}} q^{\mu}(\mathbf{x},t+\Delta t)&=\sum_{\mathbf{x}} q_i^{\mu}n^i(\mathbf{x}+\mathbf{c}^{\,i},t+\Delta t)\\ &=\sum_{\mathbf{x}} q_i^{\mu}[n^i(\mathbf{x},t)+\omega^i(n^*)]=\sum_{\mathbf{x}} q^{\mu}(\mathbf{x},t) \ ,\end{aligned}$$

so that the global sum of any conserved quantity is constant in time.

Note that the conserved quantities naturally partition the set S into equivalence classes. Two states belong to the same equivalence class if they have the same values of all the conserved quantities (that is, $s\sim s'$ if and only if $q_i^{\mu}s'^{\,i}=q_i^{\mu}s^i$ for $\mu=1,\dots,n_c$). Collisions must map states into other states of the same equivalence class. This means that the transition matrix $a(s\to s')$ is block diagonal, in that $a(s\to s')=0$ if $s\not\sim s'$. More succinctly,

$$a(s\to s')(q_i^{\mu}s'^{\,i}-q_i^{\mu}s^i)=0 \ . \tag{7}$$

Note that Eq. (6) follows immediately from Eqs. (4) and (7).

We observe in passing that some lattice gases also possess *spurious global conserved quantities.* For example, it is easily seen that lattice gases of single-speed particles on a Cartesian grid conserve all quantities separately on both checkerboard sublattices. Such spurious global conserved quantities have no analog for continuum fluids and need to be considered carefully when using lattice gases to model hydrodynamic phenomena [27–29].

E. Ensemble average

We now consider some statistical aspects of lattice-gas theory. Let us suppose that we have prepared an ensemble of lattice-gas simulations on grids of the same size, with initial conditions that are sampled from some distribution. We denote averages across this ensemble by angular brackets. We define

$$N^i(\mathbf{x},t)\equiv\langle n^i(\mathbf{x},t)\rangle \ .$$

Note that while the n^i's are binary, the N^i's take their values in the set of real numbers between zero and one. Similarly, we can consider ensemble-averaged values of the conserved quantities

$$Q^{\mu}(\mathbf{x},t)\equiv\langle q^{\mu}(\mathbf{x},t)\rangle=q_i^{\mu}N^i(\mathbf{x},t) \quad \text{for } \mu=1,\dots,n_c \ . \tag{8}$$

Next, the ensemble average of $a(s\to s')$ is defined to be

$$A(s\to s')=\langle a(s\to s')\rangle \ ,$$

so that the ensemble average of Eq. (2) is

$$\sum_{s'} A(s\to s')=1 \ . \tag{9}$$

For deterministic lattice gases, $A(s\to s')=a(s\to s')$, whereas for stochastic lattice gases, the elements of $A(s\to s')$ are generally real numbers between 0 and 1.

Note that we now have three possible levels of description of the lattice-gas system. At the finest level, the specification of the $n^i(\mathbf{x},t)$ constitutes a complete microscopic description of the system. Their time evolution can generally be obtained only by an actual simulation of the lattice gas. Often, however, precise knowledge of each and every bit of the system is more information than one really desires. A coarser description, such as a closed set of *kinetic* equations for the ensemble-averaged $N^i(\mathbf{x},t)$ is often a more appropriate description of the system. Even this level of description, however, is redundant for many purposes. Therefore, at the coarsest level, one might seek a closed set of *hydrodynamic* equations for the Q^{μ}. The remainder of this paper will be concerned with deriving these two reduced descriptions of the system.

F. Boltzmann equation

Toward the goal of obtaining a closed set of equations for the N^i, we take the ensemble average of Eq. (1). We are immediately thwarted by the fact that the collision operator, given by Eq. (4), is generally a nonlinear function of the n^i. The average of a nonlinear function is not in general expressible as a function of the averaged quantities. It also depends on the *correlations* between the quantities—in this case between the incoming bits n^i.

Thus the simplest approximation that we can make to close the system of equations for the N^i is to assume that the incoming bits n^i are uncorrelated. This is the discrete version of the famous *Boltzmann molecular chaos assumption*. From this assumption, it would follow that

$$\langle \omega^i(n^*) \rangle \approx \Omega^i(\langle n^* \rangle) = \Omega^i(N^*) ,$$

where, using Eqs. (3) and (4), $\Omega^i(N^*)$ is given by

$$\begin{aligned}\Omega^i(N^*) &= \sum_{s,s'} A(s\to s')(s'^i - s^i)\prod_{j=1}^{n}(1-s^j-N^j+2s^jN^j)\\ &= \sum_{s,s'} A(s\to s')(s'^i - s^i)\prod_{j=1}^{n}(N^j)^{s^j}(1-N^j)^{1-s^j} .\end{aligned} \tag{10}$$

In this way, we get the *lattice Boltzmann equation*

$$N^i(\mathbf{x}+\mathbf{c}^i, t+\Delta t) = N^i(\mathbf{x},t) + \Omega^i(N^*(\mathbf{x},t)) . \tag{11}$$

Physically speaking, the assumption of molecular chaos supposes that the propagation substep effectively decorrelates the different bits at each site. (For stochastic lattice gases, such decorrelation is enhanced by the injection of stochasticity at each site at each time step.) That is, it supposes that colliding particles have never had any prior effect on each other. This assumption is virtually never strictly correct for a system of particles moving on a discrete lattice in a finite number of dimensions. By standard combinatorial arguments, the reencounter probability for two particles executing a random walk on a lattice is unity in one and two dimensions, is less than unity in three or more dimensions, and falls to zero as the number of dimensions goes to infinity. Though lattice-gas particles do not execute random walks, one might still expect on these heuristic grounds that the molecular chaos assumption becomes more valid as the number of spatial dimensions increases. Indeed, this is the case and the molecular chaos assumption can be thought of as a sort of mean-field theory. In some circumstances, it is possible for particles to set up coherent structures that persist for long times. Such structures, by their very nature, invalidate the molecular chaos assumption in a rather dramatic way.

The remainder of this paper is devoted to deriving the desired closed set of hydrodynamic equations for the Q^μ. We shall go about this task in two stages. First, in Sec. III, we shall show how they can be derived under the molecular chaos assumption. In Sec. VI, however, we abandon this assumption and find that this has the effect of correcting, or *renormalizing*, the transport coefficients in the resulting hydrodynamic equations. For a large class of lattice gases of interest—those satisfying a condition known as *semidetailed balance* at lowest order—we shall show that it is possible to write an exact expression for this correction as a diagrammatic series.

III. CHAPMAN-ENSKOG ANALYSIS

A. Asymptotic ordering

We shall now outline a perturbative analysis of the Boltzmann equation (11). With this analysis, we study the hydrodynamics of systems that deviate slightly from local equilibrium conditions. To do this, we must first establish the asymptotic regime that we are trying to study. In this paper we use a scaling limit that is sometimes called *diffusion ordering* or *Navier-Stokes ordering*. This ordering can be obtained formally by letting $\mathbf{c}\to\epsilon\mathbf{c}$ and $\Delta t\to\epsilon^2\Delta t$ in the dynamical equations, where ϵ is an expansion parameter. Thus we are taking $\Delta t \sim c^2$, as is appropriate for diffusive or viscous processes.

Because the N^i are real numbers (as opposed to the n^i, which are bits), we are free to approximate them by smooth functions that happen to coincide with them in value on the lattice points. We can then Taylor expand Eq. (11), retaining terms to order ϵ^2. Dividing out Δt, we get

$$\begin{aligned}\epsilon^2\frac{\partial N^i}{\partial t} + \epsilon\nabla\cdot\left[\frac{\mathbf{c}^i}{\Delta t}N^i\right] + \epsilon^2\nabla\nabla : \left[\frac{\mathbf{c}^i\mathbf{c}^i}{2\Delta t}N^i\right]\\ = \frac{1}{\Delta t}\Omega_0^i(N^*) + \frac{\epsilon}{\Delta t}\Omega_1^i(N^*) + \frac{\epsilon^2}{\Delta t}\Omega_2^i(N^*) ,\end{aligned} \tag{12}$$

where the double-dot notation denotes two inner products. (This notation will be used only when no ambiguity can arise from it, as is the case when at least one of the two dyads involved is symmetric.) Note that we have ordered the ensemble-averaged collision operator in the expansion parameter ϵ. This is useful for lattice gases with collision rules that depend upon the lattice size; for example, the collision rule for the Burgers equation lattice gas, which we shall describe later in this paper, has a directional bias that is proportional to ϵ in the scaling limit. In what follows, we shall assume that Ω_0^i and Ω_1^i respect the conservation laws exactly, but that Ω_2^i does not necessarily do so. This will allow us to consider lattice gases whose conservation laws are only approximate.

Contracting Eq. (12) with the constant q_i^μ, we get the n_c conservation equations

$$\begin{aligned}\epsilon\frac{\partial Q^\mu}{\partial t} + \nabla\cdot\left[\left[q_i^\mu\frac{\mathbf{c}^i}{\Delta t}N^i\right] + \epsilon\nabla\cdot\left[q_i^\mu\frac{\mathbf{c}^i\mathbf{c}^i}{2\Delta t}N^i\right]\right]\\ = \frac{\epsilon}{\Delta t}q_i^\mu\Omega_2^i(N^*) ,\end{aligned} \tag{13}$$

where $\mu=1,\ldots,n_c$. We can now clearly identify the quantity in square brackets as the flux corresponding to the conserved density Q^μ and the right-hand side as a source or sink term.

In what follows, we shall expand the N^i in a perturbation series in powers of ϵ about an equilibrium state,

$$N^i = N_0^i + \epsilon N_1^i + \epsilon^2 N_2^i + \cdots . \tag{14}$$

Here N_0^i is a local thermodynamic equilibrium. In the next subsection, we shall characterize these equilibria. Then we shall derive hydrodynamic equations for the system by considering its near-equilibrium behavior.

B. Semidetailed balance and equilibria

An *equilibrium distribution* for a given lattice gas is a distribution on the state space of the system that is invariant under the full dynamics. A *Boltzmann equilibri-*

um is a set of values for the mean occupation numbers N^a, which is invariant under the Boltzmann equation (11). A Boltzmann equilibrium can be associated with a distribution on the set of states by independently sampling each bit n^a with probability N^a. If the resulting distribution is an equilibrium in the more general sense, then we refer to this distribution as a *Gibbsian equilibrium.* Thus, in a Gibbsian equilibrium the full dynamics of the system, given by Eq. (1), do not generate correlations between the n^a. If a Boltzmann equilibrium is spatially uniform, it can be specified by a set of values for the n mean occupation numbers N^i; the associated distribution on the set of states is given by independently sampling each bit n^a with probability $N^{i(a)}$.

We wish to study the dynamics of the system in the vicinity of a local Boltzmann equilibrium. Inserting Eq. (14) into Eq. (12), we have at lowest order in ϵ

$$\Omega_0^i(N_0^*(\mathbf{x},t))=0 , \tag{15}$$

which is the condition that the N_0^i are a Boltzmann equilibrium at $O(1)$. We also demand that the N_0^i be a Gibbsian equilibrium at this order. However, we shall allow the $N_0^i(\mathbf{x},t)$ to have spatial dependence. In this paper, we shall restrict our attention to lattice gases for which equilibria with these properties exist. Fortunately, this restriction can be formulated in terms of a simple sufficient condition on the lowest-order part of the transition matrix [2]. To state this condition, we first introduce a definition.

Definition 1. A lattice gas is said to obey *detailed balance* if its transition matrix satisfies

$$A(s\rightarrow s')=A(s'\rightarrow s) \tag{16}$$

and it is said to obey *semidetailed balance* if its transition matrix satisfies

$$\sum_s A(s\rightarrow s')=1 . \tag{17}$$

Note that semidetailed balance is a weaker condition than detailed balance, because Eqs. (16) and (9) together imply Eq. (17). Semidetailed balance (coupled with probability conservation) requires that the rows and columns of the transition matrix all sum to unity. Detailed balance additionally requires that it be symmetric. For a deterministic lattice gas, detailed balance requires that if the transition matrix takes state s to state s', then it must also take state s' to state s. In this case, semidetailed balance is the weaker condition that the final states are a permutation of the initial states.

We now quote [2] and prove a theorem due to Hénon on the existence of Gibbsian equilibria.

Theorem 1. Spatially uniform Gibbsian equilibria exist for any lattice gas obeying semidetailed balance. These equilibria are described by the Fermi-Dirac distribution

$$N_0^i=\frac{1}{1+\exp\left[-\sum_{\mu=1}^{n_c}\alpha_\mu q_i^\mu\right]} , \tag{18}$$

where the α_μ are n_c arbitrary multipliers.

Proof. At first, Eq. (15) appears to impose n conditions on the n unknowns N_0^i, but the n_c restrictions imposed by Eq. (6) mean that only $n-n_c$ of these conditions are independent and therefore that we ought to expect an n_c parameter family of equilibria. These will be the constants α_μ in Eq. (18).

Taking the Fermi-Dirac distribution (18) to define an independent distribution on the bits of the system, the probability at any site of a fixed state s is given by

$$P_0(s)=\prod_{j=1}^{n}(N_0^j)^{s^j}(1-N_0^j)^{1-s^j} . \tag{19}$$

In order to show that this distribution on states defines an equilibrium, we must show that the distribution is unchanged by the collision operator. From the block diagonal property (7) of the transition matrix and the property of semidetailed balance, it is clear that it will suffice to prove that the probability (19) is dependent only on the equivalence class of s and therefore on the quantities $q_i^\mu s^i$ for $\mu=1,\ldots,n_c$. Inserting Eq. (18) into Eq. (19), we have

$$P_0(s)=\frac{\exp\left[-\sum_{\mu=1}^{n_c}\alpha_\mu\sum_i q_i^\mu(1-s^i)\right]}{\prod_i\left[1+\exp\left[-\sum_{\mu=1}^{n_c}\alpha_\mu q_i^\mu\right]\right]} .$$

This expression indeed only depends upon the equivalence class of the state s and therefore we have proven that the distribution on states defined by Eq. (18) is a Gibbsian equilibrium. ■

The equilibrium distribution given by Eq. (18) is an n_c-parameter family of solutions for the N_0^i. By taking the parameters α_μ to be spatially dependent, we can construct a family of equilibria that generates correlations only at $O(\epsilon)$. These are precisely the type of spatially varying equilibria that we desire for the lowest-order means N_0^i of our lattice gas. Thus, in what follows we restrict our attention to lattice gases that obey semidetailed balance at lowest order.

Summarizing the constraints on the collision operator at each order, we have the following: Ω_0^i must respect the conservation laws and obey semidetailed balance; Ω_1^i must respect the conservation laws, but may violate semidetailed balance; Ω_2^i can violate either the conservation laws or semidetailed balance.

Finally, we note that since the parameters α_μ are arbitrary multipliers, any set of n_c independent functions of them would also suffice to parametrize the equilibrium. In particular, a natural and logical choice of parameters are the hydrodynamic densities Q^μ. These can be related to the α_μ by their definition Eq. (8),

$$Q^\mu=q_i^\mu N_0^i(\alpha_*) \text{ for } \mu=1,\ldots,n_c . \tag{20}$$

Thus the equilibrium distribution N_0^i can be parametrized solely by the equilibrium values of the n_c conserved densities.

C. Fermi metric

In what follows, we shall need the first two derivatives of the N_0^i with respect to the Q^μ, so we compute them here by the chain rule. First, by differentiating Eq. (18) with respect to α_ν, we obtain

$$\frac{\partial N_0^i}{\partial \alpha_\nu} = N_0^i(1-N_0^i)q_i^\nu \tag{21}$$

(where there is no summation over i because it appears only once on the left). Next, by differentiating Eq. (20) with respect to Q^ν, we obtain

$$\delta^\mu{}_\nu = \sum_{\xi=1}^{n_c} q_j^\mu \frac{\partial N_0^j}{\partial \alpha_\xi}\frac{\partial \alpha_\xi}{\partial Q^\nu} = \sum_{\xi=1}^{n_c} g^{\mu\xi}\frac{\partial \alpha_\xi}{\partial Q^\nu} ,$$

where we have defined the symmetric rank-two tensor

$$g^{\mu\xi} \equiv N_0^j(1-N_0^j)q_j^\mu q_j^\xi . \tag{22}$$

We denote the inverse of this matrix by $g_{\xi\nu}$ so that

$$\sum_{\xi=1}^{n_c} g^{\mu\xi}g_{\xi\nu} = \delta^\mu{}_\nu .$$

Since $g_{\xi\nu}$ is a symmetric second-rank tensor, we can identify it as a metric on the space of hydrodynamic variables Q^ν. We call it the *Fermi metric.* In terms of the Fermi metric, we have

$$\frac{\partial \alpha_\xi}{\partial Q^\nu} = g_{\xi\nu} .$$

Finally, we can write

$$\frac{\partial N_0^i}{\partial Q^\mu} = \sum_{\nu=1}^{n_c} N_0^i(1-N_0^i)q_i^\nu g_{\nu\mu} \tag{23}$$

(no sum on i). In similar fashion, we compute the second derivative

$$\frac{\partial^2 N_0^i}{\partial Q^\mu \partial Q^\nu} = N_0^i(1-N_0^i)(1-2N_0^i)q_i^\xi q_i^\eta g_{\xi\mu}g_{\eta\nu} + 2N_0^i(1-N_0^i)q_i^\xi g_{\xi\eta}\Gamma^\eta{}_{\mu\nu} , \tag{24}$$

where we have defined the *Fermi connection*

$$\Gamma^\eta{}_{\mu\nu} = \frac{1}{2}g^{\eta\xi}\left[\frac{\partial g_{\xi\mu}}{\partial Q^\nu} + \frac{\partial g_{\xi\nu}}{\partial Q^\mu} - \frac{\partial g_{\mu\nu}}{\partial Q^\xi}\right] = -\frac{1}{2}g_{\mu\xi}g_{\nu\zeta}N_0^j(1-N_0^j)(1-2N_0^j)q_j^\eta q_j^\xi q_j^\zeta . \tag{25}$$

Next, we introduce a characteristic lattice spacing c to define the dimensionless lattice vectors

$$\mathbf{e}^i \equiv \frac{\mathbf{c}^i}{c}$$

and consider the completely symmetric outer product of k of these vectors $\otimes^k \mathbf{e}^i$. It will be useful to include these outer products in the above sums. Thus we define the *generalized Fermi metric*

$$\mathbf{g}(k)^{\mu\xi} \equiv N_0^j(1-N_0^j)q_j^\mu q_j^\xi \left[\overset{k}{\otimes}\mathbf{e}^j\right] \tag{26}$$

and the *generalized Fermi connection*

$$\mathbf{\Gamma}(k)^\eta{}_{\mu\nu} \equiv -\tfrac{1}{2}g_{\mu\xi}g_{\nu\zeta}N_0^j(1-N_0^j)(1-2N_0^j)q_j^\eta q_j^\xi q_j^\zeta \left[\overset{k}{\otimes}\mathbf{e}^j\right]. \tag{27}$$

Note that $\mathbf{g}(0)^{\mu\xi} = g^{\mu\xi}$ and $\mathbf{\Gamma}(0)^\eta{}_{\mu\nu} = \Gamma^\eta{}_{\mu\nu}$. Once again, to raise and lower the indices of these objects, we use the Fermi metric $g_{\nu\mu}$ as a metric tensor; thus, e.g., $\mathbf{g}(2)^\xi{}_\nu = \mathbf{g}(2)^{\xi\mu}g_{\mu\nu}$.

In passing, we note that since the $\mathbf{e}^j$ are obviously independent of the Q^*, we have

$$\mathbf{\Gamma}(k)^\eta{}_{\mu\nu} = \frac{1}{2}g^{\eta\xi}\left[\frac{\partial \mathbf{g}(k)_{\xi\mu}}{\partial Q^\nu} + \frac{\partial \mathbf{g}(k)_{\xi\nu}}{\partial Q^\mu} - \frac{\partial \mathbf{g}(k)_{\mu\nu}}{\partial Q^\xi}\right]$$

for all k. That is, we have defined a set of metrics and their associated connections. For each k, the members of this set comprise a completely symmetric tensor of rank k. As we shall show, this structure is very useful for the problem at hand.

From Eqs. (23) and (24), we get

$$\frac{\partial}{\partial Q^\mu}\left[q_i^\eta N_0^i \left[\overset{k}{\otimes}\mathbf{e}^i\right]\right] = \mathbf{g}(k)^\eta{}_\mu$$

and

$$\frac{\partial^2}{\partial Q^\mu \partial Q^\nu}\left[q_i^\eta N_0^i \left[\overset{k}{\otimes}\mathbf{e}^i\right]\right] = 2[\mathbf{g}(k)^\eta{}_\xi \Gamma^\xi{}_{\mu\nu} - \mathbf{\Gamma}(k)^\eta{}_{\mu\nu}] .$$

Note that when $k=0$ these reduce to the identities $\partial Q^\eta/\partial Q^\mu = \delta^\eta{}_\mu$ and $\partial^2 Q^\eta/\partial Q^\mu \partial Q^\nu = 0$, respectively.

D. Zeroth-order conservation equations

We can now examine the conservation equation (13) at $O(1)$. We have

$$\nabla\cdot\left[q_i^\mu \frac{\mathbf{c}^i}{\Delta t}N_0^i\right] = 0 \quad \text{for } \mu = 1, \ldots, n_c . \tag{28}$$

Using Eq. (23), this can be written solely in terms of the conserved densities and their gradients. We find

$$\frac{c}{\Delta t}\sum_{\nu=1}^{n_c} \mathbf{g}(1)^\mu{}_\nu \cdot \nabla Q^\nu = 0 \quad \text{for } \mu = 1, \ldots, n_c .$$

E. Linearized Boltzmann equation

We return to Eqs. (12) and (14). At $O(\epsilon)$ we find

$$\nabla\cdot\left[\frac{\mathbf{c}^i}{\Delta t}N_0^i\right] = \frac{1}{\Delta t}[J^i{}_j N_1^j + \Omega_1^i(N_0^*)] , \tag{29}$$

where we have defined the Jacobian matrix of the lowest-order collision operator at equilibrium,

$$J^i{}_j \equiv \left.\frac{\partial \Omega_0^i}{\partial N^j}\right|_{N=N_0} .$$

By differentiating Eq. (10), we can write this directly in terms of the lowest-order transition matrix $A_0(s \to s')$ (this is the transition matrix corresponding to the lowest-order collision operator Ω_0^i),

$$J^i{}_j=\sum_{s,s'} A_0(s\rightarrow s')(s'^{\,i}-s^i)(2s^j-1) \times\prod_{k\neq j}^{n} (N_0^k)^{s^k}(1-N_0^k)^{1-s^k} . \tag{30}$$

Note that the q_i^μ's comprise the components of n_c null left eigenvectors of $J^i{}_j$, since

$$q_i^\mu J^i{}_j=\frac{\partial}{\partial N^j}(q_i^\mu\Omega_0^i)\bigg|_{N=N_0}=0 .$$

In what follows, we denote the eigenvalues of J by λ^μ. The corresponding right (left) eigenvectors are indexed as contravariant (covariant) vectors and enumerated with a subscript (superscript). Thus

$$J^i{}_j q_\mu^j=\lambda^\mu q_\mu^i \tag{31}$$

and

$$q_i^\mu J^i{}_j=\lambda^\mu q_j^\mu . \tag{32}$$

Note that, for $\mu=1,\dots,n_c$, this coincides with the definition of the q_i^μ introduced in Eq. (5).

The modes enumerated $1,\dots,n_c$ correspond to null eigenvalues of J and will be called *hydrodynamic modes;* those modes enumerated $n_c+1,\dots,n$ will be called *kinetic modes.* We shall often write H for the set $\{1,\dots,n_c\}$ and K for the set $\{n_c+1,\dots,n\}$. When the kinetic eigenvalues satisfy $\lambda^\nu<0$, we define the system to be *linearly stable.* Since the eigenvalues of J set the time scale for the equation, we see that for a linearly stable lattice gas, the kinetic modes decay away rapidly, while the hydrodynamic modes persist for long times. From Hénon's proof of Theorem 1, it follows that semidetailed balance lattice gases are linearly stable around the Gibbsian equilibrium, so they have $\lambda^\nu<0$ for $\nu\in K$.

Postmultiplying Eq. (32) by q_μ^j, premultiplying Eq. (31) by q_i^μ, and subtracting, we get

$$0=(\lambda^\beta-\lambda^\eta)q_i^\eta q_\beta^i ,$$

so that right and left eigenvectors corresponding to different eigenvalues are orthogonal. Thus they may be chosen so that

$$\delta^\mu{}_\nu=q_i^\mu q_\nu^i . \tag{33}$$

By including $\otimes^k\mathbf{e}^i$ in Eq. (33), we can define a *generalized Kronecker delta* in the same spirit that we generalized the Fermi metric and connection. Thus

$$\delta(k)^\mu{}_\nu\equiv q_j^\mu\left[\overset{k}{\otimes}\mathbf{e}^j\right]q_\nu^j , \tag{34}$$

so that $\delta(0)^\mu{}_\nu=\delta^\mu{}_\nu$. Also, note that the indices of the generalized Fermi metric and connection, as well as those of the generalized Kronecker delta, can now be extended to run over the kinetic modes as well as the hydrodynamic modes by simply using the kinetic left eigenvectors in Eqs. (26), (27), and (34), respectively.

Finally, we note that it is possible to write an explicit, closed expression for the right hydrodynamic eigenvectors. From Eqs. (15), (18), and (21), it follows immediately that

$$0=\frac{\partial}{\partial\alpha_\mu}\Omega_0^i(N_0^*)=J^i{}_j\frac{\partial N_0^j}{\partial\alpha_\mu}=J^i{}_j[q_j^\mu N_0^j(1-N_0^j)] ,$$

whence we identify the right hydrodynamic eigenvectors

$$q_\mu^i=q_i^\nu N_0^i(1-N_0^i)g_{\mu\nu} .$$

Note that this result is in accordance with Eq. (22).

F. First-order solution

Consider Eq. (29) for the N_1^i. Since J is a singular matrix, we must verify that the equation is consistent. The consistency requirement is found by premultiplying the equation by the null left eigenvectors. We obtain the requirement

$$\nabla\cdot\left[q_i^\mu\frac{\mathbf{c}^i}{\Delta t}N_0^i\right]=\frac{1}{\Delta t}q_i^\mu[J^i{}_jN_1^j+\Omega_1^i(N_0^*)]=0$$

for $\mu\in H$. Note that this consistency requirement is precisely the zeroth-order conservation equation (28). It follows that $\nabla\cdot(\mathbf{c}^iN_0^i)-\Omega_1^i(N_0^*)$ has no components in the null space of J. Thanks to the completeness and orthonormality of the eigenvectors, this expression can be written as

$$\nabla\cdot(\mathbf{c}^iN_0^i)-\Omega_1^i(N_0^*)=\sum_{\nu\in K}\eta^\nu q_\nu^i ,$$

where

$$\eta^\nu\equiv q_j^\nu[\nabla\cdot(\mathbf{c}^jN_0^j)-\Omega_1^j(N_0^*)] \quad \text{for } \nu\in K .$$

The solution for N_1^i can then be written down immediately,

$$N_1^i=\sum_{\nu\in H}\theta^\nu q_\nu^i+\sum_{\nu\in K}\frac{\eta^\nu}{\lambda^\nu}q_\nu^i ,$$

where the θ^ν are arbitrary. We fix the solution by assuming, without loss of generality, that $\theta^\nu=0$. That is, we assume that the first-order contribution does not affect the definitions of the conserved densities. The final result for the N_1^i is then

$$N_1^i=\sum_{\nu\in K}\frac{q_\nu^iq_j^\nu}{\lambda^\nu}[\nabla\cdot(\mathbf{c}^jN_0^j)-\Omega_1^j(N_0^*)] , \tag{35}$$

so that we have

$$N^i=N_0^i+\epsilon\sum_{\nu\in K}\frac{q_\nu^iq_j^\nu}{\lambda^\nu}[\nabla\cdot(\mathbf{c}^jN_0^j)-\Omega_1^j(N_0^*)]+O(\epsilon^2) . \tag{36}$$

G. First-order conservation equations

We now insert Eq. (36) into the conservation equation (13), retaining terms to $O(\epsilon)$. After some manipulation, we get the following closed set of equations for the conserved densities:

$$\frac{\partial Q^\mu}{\partial t}+\nabla\cdot\mathcal{A}^{\mu}=\sum_{\xi\in H}\nabla\cdot(\mathcal{D}^{\mu}{}_{\xi}\cdot\nabla Q^{\xi})+\mathcal{S}^{\mu}\quad\text{for }\mu\in H\ , \tag{37}$$

where the advection coefficient, the diffusion coefficient, and the source term are given by

$$\mathcal{A}^{\mu}(Q^*)\equiv\frac{c}{\Delta t}\sum_{\nu\in K}\frac{\boldsymbol{\delta}(1)^{\mu}{}_{\nu}\mathcal{C}_1^{\nu}(Q^*)}{(-\lambda^\nu)}\ , \tag{38}$$

$$\mathcal{D}^{\mu}{}_{\xi}(Q^*)\equiv\frac{c^2}{\Delta t}\left[\sum_{\nu\in K}\frac{\boldsymbol{\delta}(1)^{\mu}{}_{\nu}\otimes\mathbf{g}(1)^{\nu}{}_{\xi}}{(-\lambda^\nu)}-\frac{1}{2}\mathbf{g}(2)^{\mu}{}_{\xi}\right]\ , \tag{39}$$

$$\mathcal{S}^{\mu}(Q^*)\equiv\frac{1}{\Delta t}\mathcal{C}_2^{\mu}(Q^*)\ , \tag{40}$$

respectively, and where

$$\mathcal{C}_n^{\mu}(Q^*)\equiv q_i^{\mu}\Omega_n^i(N_0^*(Q^*))\quad\text{for }n=1,2\ . \tag{41}$$

The compact form of this result makes it straightforward to compute the transport coefficients of any lattice gas. Note that knowledge of the conserved quantities and the concomitant hydrodynamic modes is sufficient to predict the form of this equation.

H. Ordering the conserved quantities

There is one additional technicality that we need to discuss before presenting examples of this formalism. In many situations of interest, the conserved quantities themselves are ordered in the expansion parameter ϵ. For example, in an incompressible fluid, the hydrodynamic density is assumed to vary by $O(\epsilon^2)$ from a constant background value and the hydrodynamic velocity is assumed to be $O(\epsilon)$ (low Mach number).

Consider the general ordering

$$Q^{u}=Q_0^{\mu}+\epsilon Q_1^{\mu}+\epsilon^2 Q_2^{\mu}+\cdots\ , \tag{42}$$

where it is assumed that the zeroth-order value Q_0^μ is always independent of position and time. We can then expand the Fermi-Dirac equilibrium as

$$\begin{aligned}N_0^i(Q^*)&=N_0^i(Q_0^*)+\sum_{\mu\in H}\left.\frac{\partial N_0^i}{\partial Q^\mu}\right|_0(\epsilon Q_1^\mu+\epsilon^2 Q_2^\mu)+\frac{1}{2}\sum_{\mu,\nu\in H}\left.\frac{\partial N_0^i}{\partial Q^\mu\partial Q^\nu}\right|_0(\epsilon^2 Q_1^\mu Q_1^\nu)+\cdots\\&=N_{00}^i+\epsilon\sum_{\xi\in H}N_{00}^i(1-N_{00}^i)q_i^{\xi}g_{\xi\mu}Q_1^\mu\\&\quad+\epsilon^2\left[\sum_{\xi\in H}N_{00}^i(1-N_{00}^i)q_i^{\xi}g_{\xi\mu}Q_2^\mu+\sum_{\xi,\eta\in H}N_{00}^i(1-N_{00}^i)q_i^{\xi}g_{\xi\eta}\Gamma^{\eta}{}_{\mu\nu}Q_1^\mu Q_1^\nu\right.\\&\quad\left.+\frac{1}{2}\sum_{\xi,\eta\in H}N_{00}^i(1-N_{00}^i)(1-2N_{00}^i)q_i^{\xi}q_i^{\eta}g_{\xi\mu}g_{\eta\nu}Q_1^\mu Q_1^\nu\right]+\cdots\ ,\end{aligned}$$

where we have defined the lowest-order Chapman-Enskog equilibrium

$$N_{00}^i\equiv N_0^i(Q_0^*)$$

and we note that the Fermi metrics and connections in the above expression are now defined in terms of N_{00}^i rather than N_0^i.

To make it possible to incorporate this sort of ordering into the above formalism, we return to the Chapman-Enskog solution for the Boltzmann distribution, Eq. (36), insert the above expansion of $N_0^i(Q^*)$, multiply by the k-fold outer product of the $\mathbf{e}^i$ vectors, and contract with q_i^μ. In the interest of simplifying the algebra a bit, we shall assume that $\Omega_1^i=0$ in this subsection; we do, however, continue to include Ω_2^i in our analysis. The assumption that $\Omega_1^i=0$ is not in any way essential, but it serves to keep the algebra in check. We get

$$\begin{aligned}&q_i^\mu\left[\overset{k}{\otimes}\mathbf{e}^i\right]N^i(Q^*)\\&\quad=q_i^\mu\left[\overset{k}{\otimes}\mathbf{e}^i\right]N_{00}^i+\sum_{\xi\in H}\mathbf{g}(k)^{\mu}{}_{\xi}(\epsilon Q_1^\xi+\epsilon^2 Q_2^\xi)\\&\qquad+\epsilon^2\sum_{\xi,\eta\in H}\left[\sum_{\zeta\in H}\mathbf{g}(k)^{\mu}{}_{\zeta}\Gamma^{\zeta}{}_{\xi\eta}-\boldsymbol{\Gamma}(k)^{\mu}{}_{\xi\eta}\right]Q_1^\xi Q_1^\eta\\&\qquad+\epsilon^2 c\sum_{\nu\in K}\sum_{\xi\in H}\frac{\boldsymbol{\delta}(k)^{\mu}{}_{\nu}\otimes\mathbf{g}(1)^{\nu}{}_{\xi}}{\lambda^\nu}\cdot\nabla Q_1^\xi\ .\end{aligned}$$

This result can be directly inserted in the conservation equation (13), retaining terms to $O(\epsilon^2)$. After canceling a factor of ϵ^2 throughout the equation, we get

$$\frac{\partial Q_1^\mu}{\partial t}+\nabla\cdot\mathcal{A}^{\mu}=\sum_{\xi\in H}\nabla\cdot(\mathcal{D}^{\mu}{}_{\xi}\cdot\nabla Q_1^{\xi})+\mathcal{S}^{\mu}\quad\text{for }\mu\in H\ , \tag{43}$$

where we have defined the advection coefficient

$$\begin{aligned}\mathcal{A}^{\mu}(Q_0^*)\equiv\frac{c}{\Delta t}\sum_{\xi\in H}\Bigg\{&\mathbf{g}(1)^{\mu}{}_{\xi}\left[\frac{1}{\epsilon}Q_1^\xi+Q_2^\xi\right]\\&+\sum_{\eta\in H}\left[\sum_{\zeta\in H}\mathbf{g}(1)^{\mu}{}_{\zeta}\Gamma^{\zeta}{}_{\xi\eta}-\boldsymbol{\Gamma}(1)^{\mu}{}_{\xi\eta}\right]\\&\times Q_1^\xi Q_1^\eta\Bigg\}\ ,\end{aligned} \tag{44}$$

where the diffusion coefficient and source term are still given by Eqs. (39) and (40), respectively, and where all quantities are now understood to be evaluated at N_{00}^i. Note that the diffusion coefficient is now a function only of Q_0^* and hence strictly independent of space and time. The advection coefficient, on the other hand, is generally quadratic in Q_1 and linear in Q_2.

Also note that the advection coefficient has an $O(1/\epsilon)$

term and an $O(1)$ term. If the $O(1/\epsilon)$ term does not vanish, it is the dominant term in the equation. In this situation, the hydrodynamic equation reduces to the zeroth-order conservation equation

$$\nabla\cdot\left[\frac{c}{\Delta t}\sum_{\xi\in H}\mathbf{g}(1)^{\mu}{}_{\xi}Q^{\xi}_{1}\right]=0\ . \tag{45}$$

Finally, note that knowledge of the conservation laws and concomitant hydrodynamic modes is sufficient to predict the form of this equation *and* compute the advection coefficient. Only the computation of the diffusion coefficient requires knowledge of the kinetic modes in this ordering scheme.

IV. EXAMPLES OF THE BOLTZMANN-CHAPMAN-ENSKOG ANALYSIS

In this section, we present four examples of the Boltzmann–Chapman-Enskog formalism described in the previous two sections. In each case, we work out the form of the hydrodynamic equation and the transport coefficient(s) predicted by the theory.

The first example is a one-dimensional, stochastic, diffusive lattice gas with three particles per site (1D3P). The second is a lattice gas for Burgers's equation [8] in one dimension. The third is a two-dimensional lattice gas with four particles per site (2D4P) giving rise to coupled diffusion equations. Finally, we consider lattice fluid models; we consider a general class of such models and describe in detail a particular model, the FHP-I lattice gas fluid. For all but the first of these examples the Chapman-Enskog method has already been carried out. Our purpose, however, is to use these as sample applications of our general formalism and as examples for which we shall study the exact dynamics later in this paper. After presenting the complete lattice gas kinetic theory in Sec. VI, we shall return to these examples in Sec. VII, discuss observed discrepancies from the Boltzmann theory, and show how they are explained by the present theory. As we shall see, each example has its own unique and interesting features in this regard.

A. 1D3P lattice gas

As a first example, we consider a diffusive lattice-gas model in one dimension ($D=1$). The model has three bits per site ($n=3$), corresponding to the presence or absence of left-moving, stationary, and right-moving particles, respectively. These bits are denoted by the respective elements of the set $B=\{-,0,+\}$. Collisions occur only if exactly two particles enter a site. If we denote the two-particle states by $\hat{+}\equiv\{-,0\}$, $\hat{0}\equiv\{-,+\}$, and $\hat{-}\equiv\{0,+\}$, then the nontrivial elements of the state transition table can be written

$a(s\rightarrow s')$		s'	
s	$\hat{+}$	$\hat{0}$	$\hat{-}$
$\hat{+}$	$1-n^p$	$n^p(1-n^r)$	n^pn^r
$\hat{0}$	n^pn^r	$1-n^p$	$n^p(1-n^r)$
$\hat{-}$	$n^p(1-n^r)$	n^pn^r	$1-n^p$

The bits n^p and n^r are random bits, which are sampled separately at each lattice site and at each time step with average values $\langle n^p\rangle=2p$ and $\langle n^r\rangle=\frac{1}{2}$. (Note that r and p are not indices here, but simply labels for the random bits.) Here the parameter $p\in[0,\frac{1}{2}]$ may be thought of as the probability of collision from, e.g., $\hat{+}$ to $\hat{0}$. The value of the bit n^p effectively determines whether or not a collision will occur and that of n^r determines which of the two possible outcomes will result.

Note that these collisions conserve particles ($n_c=1$); it is the particle density that obeys the macroscopic diffusion equation. The coefficients q^1_* for the conserved quantity are

$$q^1_-=q^1_0=q^1_+=1\ . \tag{46}$$

The collision operator is given by Eq. (4),

$$\omega^i(n^*)=n^p[\overline{n^i}n^{i+1}n^{i+2}-\overline{n^r}n^i\overline{n^{i+1}}n^{i+2}-n^rn^in^{i+1}\overline{n^{i+2}}] \tag{47}$$

for each $i\in B$, where $\overline{n^i}\equiv 1-n^i$ denotes the complement of a bit and where the addition of integers to i is understood to increment i through the set B in cyclic fashion. According to Eq. (6), we observe that

$$0=\omega^-+\omega^0+\omega^+\ .$$

We now consider the ensemble average of this system. The ensemble-averaged state transition table is

$A(s\rightarrow s')$		s'	
s	$\hat{+}$	$\hat{0}$	$\hat{-}$
$\hat{+}$	$1-2p$	p	p
$\hat{0}$	p	$1-2p$	p
$\hat{-}$	p	p	$1-2p$

Note that semidetailed balance is satisfied since the columns of the above table sum to unity. Also note that the ensemble-averaged collision operator in the Boltzmann approximation is given by Eq. (10), which reads

$$\Omega^i(N^*)=2pN^{i+1}N^{i+2}-pN^iN^{i+1}-pN^iN^{i+2}\ .$$

We do not order the collision operator in this lattice gas, so that $\Omega^i=\Omega^i_0$. Using Eq. (46), we calculate the local Fermi-Dirac equilibrium from Eq. (18),

$$N^-_0=N^0_0=N^+_0=\frac{1}{1+e^{-\alpha}}\equiv f\ , \tag{48}$$

where α parametrizes the distribution function and f is the mean occupation number. Note that the total density is given in terms of α (and f) by

$$Q=\frac{3}{1+e^{-\alpha}}=3f\ ,$$

which is the analog of Eq. (20).

We now perform the Chapman-Enskog perturbative analysis. The Jacobian of the collision operator at equilibrium is

$$J=\begin{bmatrix} -2pf & pf & pf \\ pf & -2pf & pf \\ pf & pf & -2pf \end{bmatrix} . \tag{49}$$

This matrix has eigenvalues

$$\lambda^1=0$$

and

$$\lambda=\lambda^2=\lambda^3=-3pf ,$$

with corresponding left eigenvectors

$$\begin{aligned} q^1&=(+1 \quad +1 \quad +1) , \\ q^2&=(-1 \quad 0 \quad +1) , \\ q^3&=(-1 \quad +2 \quad -1) \end{aligned} \tag{50}$$

and right eigenvectors

$$q_1=\tfrac{1}{3}\begin{bmatrix}+1\\+1\\+1\end{bmatrix},\quad q_2=\tfrac{1}{2}\begin{bmatrix}-1\\0\\+1\end{bmatrix},\quad q_3=\tfrac{1}{6}\begin{bmatrix}-1\\+2\\-1\end{bmatrix} .$$

It is easy to check that these eigenvectors satisfy Eq. (33).

We may now construct the Fermi metric. There is only one hydrodynamic mode, so $g^{\mu\nu}$ is a 1×1 matrix. From Eq. (22) we see that its element is

$$g^{11}=3f(1-f)$$

and hence

$$g_{11}=\frac{1}{3f(1-f)} .$$

To get the generalized Fermi metric, we write $\mathbf{c}^i=c\mathbf{e}^i$, where

$$\mathbf{e}^-=-\hat{\mathbf{x}},\quad \mathbf{e}^0=\mathbf{0},\quad \mathbf{e}^+=+\hat{\mathbf{x}} ,$$

with $\hat{\mathbf{x}}$ being a unit vector and c the lattice spacing. Using Eq. (50) in Eq. (26), it follows that

$$\mathbf{g}(1)^{11}=\mathbf{0},\quad \mathbf{g}(1)^{21}=2f(1-f)\hat{\mathbf{x}},\quad \mathbf{g}(1)^{31}=\mathbf{0}$$

and

$$\begin{aligned} \mathbf{g}(2)^{11}&=+2f(1-f)\hat{\mathbf{x}}\hat{\mathbf{x}} , \\ \mathbf{g}(2)^{21}&=\mathbf{0} , \\ \mathbf{g}(2)^{31}&=-2f(1-f)\hat{\mathbf{x}}\hat{\mathbf{x}} . \end{aligned}$$

Using g_{11} to lower indices, we find

$$\mathbf{g}(1)^1{}_1=\mathbf{0},\quad \mathbf{g}(1)^2{}_1=\tfrac{2}{3}\hat{\mathbf{x}},\quad \mathbf{g}(1)^3{}_1=\mathbf{0}$$

and

$$\mathbf{g}(2)^1{}_1=+\tfrac{2}{3}\hat{\mathbf{x}}\hat{\mathbf{x}},\quad \mathbf{g}(2)^2{}_1=\mathbf{0},\quad \mathbf{g}(2)^3{}_1=-\tfrac{2}{3}\hat{\mathbf{x}}\hat{\mathbf{x}} .$$

Finally, the generalized Kronecker delta $\delta(1)^{\mu}{}_{\nu}$, given by Eq. (34), has components

$$\delta(1)^1{}_2=\hat{\mathbf{x}},\quad \delta(1)^1{}_3=\mathbf{0} .$$

The conserved quantity Q is not ordered, so we can use the results of Sec. III G. The collision operator was not ordered, so $\mathcal{C}^{\nu}_1=\mathcal{C}^{\nu}_2=0$; Eq. (37) thus tells us that there is no advection or source term in the final hydrodynamic equation. The diffusivity is given by Eq. (39),

$$\begin{aligned} \mathcal{D}^1{}_1&=\frac{c^2}{\Delta t}\left[\sum_{\nu\in K}\frac{\delta(1)^1{}_\nu\otimes\mathbf{g}(1)^\nu{}_1}{(-\lambda^\nu)}-\frac{1}{2}\mathbf{g}(2)^1{}_1\right] \\ &=\frac{c^2}{3\Delta t}\left[\frac{2}{-\lambda}-1\right]\hat{\mathbf{x}}\hat{\mathbf{x}}=\mathcal{D}\hat{\mathbf{x}}\hat{\mathbf{x}} . \end{aligned}$$

Writing $\nabla=\hat{\mathbf{x}}\partial/\partial x$, Eq. (37) gives us the hydrodynamic equation

$$\frac{\partial f}{\partial t}=\frac{\partial}{\partial x}\left[\mathcal{D}\frac{\partial f}{\partial x}\right] ,$$

where the scalar diffusivity is

$$\mathcal{D}\equiv\frac{c^2}{3\Delta t}\left[\frac{2}{-\lambda}-1\right]=\frac{c^2}{3\Delta t}\left[\frac{2}{3pf}-1\right] .$$

Since p lies in $[0,\frac{1}{2}]$ and f lies in $[0,1]$, it follows that $\mathcal{D}$ is always positive.

B. The Burgers equation lattice gas

The next example is a lattice gas for the one-dimensional ($D=1$) Burgers equation [8]. This model has two bits per site ($n=2$) corresponding to particles moving left and right. The bits are denoted by the elements of the set $B=\{-,+\}$. Collisions occur only when exactly one particle enters a site, from either direction. The result of a collision is then one particle leaving to the left (state $\{-\}$) with probability $(1-a)/2$ or to the right (state $\{+\}$) with probability $(1+a)/2$, regardless of the direction of the incoming particle.

The state transition table is thus given by

$a(s\to s')$	s'	
s	$-$	$+$
$-$	$1-n^r$	n^r
$+$	$1-n^r$	n^r

where n^r is a random bit with mean $\langle n^r\rangle=(1+a)/2$. Note that particles are conserved, so

$$q^1_-=q^1_+=1 .$$

The collision operator is given by Eq. (4),

$$\omega^{\pm}(n^*)=\pm[n^r\overline{n^+}n^- - \overline{n^r}n^+\overline{n^-}] .$$

We observe that, in accordance with Eq. (6),

$$0=\omega^-+\omega^+ .$$

The ensemble-averaged state transition table is

$A(s\to s')$	s'	
s	$-$	$+$
$-$	$(1-a)/2$	$(1+a/2)$
$+$	$(1-a)/2$	$(1+a/2)$

and the ensemble-averaged collision operator in the Boltzmann approximation is given by Eq. (10), which reads

$$\Omega^{\pm}(N^*)=\pm\left[\frac{1+a}{2}(1-N^+)N^- - \frac{1-a}{2}N^+(1-N^-)\right] .$$

Note that the collisions do not satisfy semidetailed balance unless $a=0$. We therefore restrict attention to small values of the bias $[a \sim O(\epsilon)]$ and order the Boltzmann collision operator as

$$\Omega_0^{\pm}(N^*)=\pm\tfrac{1}{2}(N^- - N^+) ,$$

$$\Omega_1^{\pm}(N^*)=\pm\frac{a}{2}(N^- + N^+)\mp aN^-N^+ .$$

Note that both $\Omega_0^{\pm}$ and $\Omega_1^{\pm}$ conserve particles exactly and that $\Omega_0^{\pm}$ satisfies semidetailed balance.

The local Fermi-Dirac equilibrium is given by

$$N_0^{\pm}=\frac{1}{1+e^{-\alpha}}\equiv f ,$$

where α parametrizes the distribution function and f is the mean occupation number. The total density is given in terms of α (and f) by

$$Q=\frac{2}{1+e^{-\alpha}}=2f .$$

The Jacobian of the collision operator at equilibrium is

$$J=\begin{bmatrix} -\frac{1}{2} & +\frac{1}{2} \\ +\frac{1}{2} & -\frac{1}{2} \end{bmatrix} .$$

This matrix has eigenvalues

$$\lambda^1=0, \quad \lambda^2=-1 ,$$

with corresponding left eigenvectors

$$q^1=(+1 \quad +1) ,$$

$$q^2=(+1 \quad -1)$$

and right eigenvectors

$$q_1=\tfrac{1}{2}\begin{bmatrix} +1 \\ +1 \end{bmatrix}, \quad q_2=\tfrac{1}{2}\begin{bmatrix} +1 \\ -1 \end{bmatrix} .$$

Once again, it is easy to check that these eigenvectors satisfy Eq. (33).

Again, there is only one hydrodynamic mode. The components of the Fermi metric and generalized Kronecker delta are readily calculated, as in the previous example. Once again, the conserved quantity Q is not ordered, so we can use the results of Sec. III G. This time, however, the collision operator is ordered. The first-order collision operator respects the conserved quantity, as required, so $\mathcal{C}_1^1=0$. The component $\mathcal{C}_1^2$, on the other hand, is nonzero, so there will be an advective term in the hydrodynamic equation. From Eq. (41), we find

$$\mathcal{C}_1^2=a(N_0^+ + N_0^- - 2N_0^+N_0^-)=2af(1-f)=aQ\left[1-\frac{Q}{2}\right].$$

The advection coefficient is given by Eq. (38),

$$\mathcal{A}^{\mu}(Q^*)=\frac{c}{\Delta t}\sum_{\nu\in K}\frac{\delta(1)^{\mu}{}_{\nu}\mathcal{C}_1^{\nu}(Q^*)}{(-\lambda^{\nu})}=\frac{ac}{\Delta t}Q\left[1-\frac{Q}{2}\right]\hat{\mathbf{x}} ,$$

and the diffusivity is given by Eq. (39),

$$\mathcal{D}^1{}_1=\frac{c^2}{\Delta t}\left[\sum_{\nu\in K}\frac{\delta(1)^1{}_{\nu}\otimes\mathbf{g}(1)^{\nu}{}_1}{(-\lambda^{\nu})}-\frac{1}{2}\mathbf{g}(2)^1{}_1\right]=\frac{c^2}{2\Delta t}\hat{\mathbf{x}}\hat{\mathbf{x}} .$$

Writing $\nabla=\hat{\mathbf{x}}\partial/\partial x$, Eq. (37) gives us the hydrodynamic equation

$$\frac{\partial Q}{\partial t}+\frac{\partial\mathcal{A}}{\partial x}=\frac{\partial}{\partial x}\left[\mathcal{D}\frac{\partial Q}{\partial x}\right] ,$$

where the scalar advection coefficient is

$$\mathcal{A}\equiv\frac{ac}{\Delta t}Q\left[1-\frac{Q}{2}\right]$$

and the scalar diffusivity is

$$\mathcal{D}\equiv\frac{c^2}{2\Delta t} .$$

Finally, if we make the change of variables $u\equiv(ac/\Delta t)(1-Q)$, this becomes Burgers's equation in the more familiar form

$$\frac{\partial u}{\partial t}+u\frac{\partial u}{\partial x}=\mathcal{D}\frac{\partial^2 u}{\partial x^2} .$$

C. 2D4P lattice gas

Next, we consider a diffusive lattice-gas model [30,31] in two spatial dimensions ($D=2$). The lattice for this model is the standard two-dimensional Cartesian lattice. The lattice gas has four bits per site ($n=4$), corresponding to the presence or absence of particles moving along each of the four unit vectors in the lattice, which we refer to as east, north, west, and south. These bits are denoted by the elements of the set $B=\{1,2,3,4\}$, respectively. Collisions occur if and only if exactly two particles enter a site at right angles and are effected by taking the complement of all four bits at such a site. For convenience, we use a diagrammatic notation for the set of states $S=\{s\subseteq B\}$. In this diagrammatic notation, each nonzero bit in a state s is denoted by a line segment emanating from a common vertex. Thus, for example, the state $s=\{2,3\}$ would be denoted by the symbol ┘ Using this notation, the nontrivial elements of the state transition table can be written

$a(s \to s')$		s'			
		└	┘	┐	┌
s	└	0	0	1	0
	┘	0	0	0	1
	┐	1	0	0	0
	┌	0	1	0	0

This collision rule separately conserves the number of east-west moving particles and the number of north-south moving particles ($n_c=2$). Thus the coefficients q_*^1 and q_*^2 for the conserved quantities are given by

$$\begin{aligned} &q_1^1=q_3^1=1,\quad q_2^1=q_4^1=0\ ,\\ &q_2^2=q_4^2=1,\quad q_1^2=q_3^2=0\ . \end{aligned} \tag{51}$$

The collision operator is given by Eq. (4),

$$\begin{aligned} \omega^i(n^*)&=\overline{n^i}\,\overline{n^{i+1}}n^{i+2}n^{i+3}+\overline{n^i}n^{i+1}n^{i+2}\overline{n^{i+3}}\\ &\quad-n^in^{i+1}\overline{n^{i+2}}\,\overline{n^{i+3}}-n^i\overline{n^{i+1}}\,\overline{n^{i+2}}n^{i+3}\\ &=(n^{i+2}-n^i)(n^{i+1}+n^{i+3}-n^{i+1}n^{i+3})\ , \end{aligned}$$

where $i\in B$ and the addition of integers to i is taken mod 4. Since the lattice gas is deterministic, we have $A(s\to s')=a(s\to s')$ and the ensemble-averaged collision operator in the Boltzmann approximation is given by $\Omega^i=\omega^i$, that is,

$$\begin{aligned} \Omega^i(N^*)&=\Omega_0^i(N^*)\\ &=(N^{i+2}-N^i)(N^{i+1}+N^{i+3}-N^{i+1}N^{i+3})\ . \end{aligned}$$

This lattice gas obeys semidetailed balance since the columns of the state transition table sum to unity. In fact, the lattice gas obeys detailed balance since the transition matrix is symmetric. Using Eqs. (51), we calculate the local Fermi-Dirac equilibrium from Eq. (18),

$$\begin{aligned} N_0^1=N_0^3&=\frac{1}{1+e^{-\alpha_1}}\equiv\mu\ ,\\ N_0^2=N_0^4&=\frac{1}{1+e^{-\alpha_2}}\equiv\nu\ , \end{aligned}$$

where α_1 and α_2, or equivalently μ and ν, parametrize the equilibrium distribution function. The east-west and north-south densities are given by

$$Q^1=\frac{2}{1+e^{-\alpha_1}}=2\mu,\quad Q^2=\frac{2}{1+e^{-\alpha_2}}=2\nu\ .$$

We now perform the Chapman-Enskog perturbative analysis. The Jacobian of the collision operator at equilibrium is

$$J=\begin{bmatrix} -\Lambda(\nu) & 0 & +\Lambda(\nu) & 0\\ 0 & -\Lambda(\mu) & 0 & +\Lambda(\mu)\\ +\Lambda(\nu) & 0 & -\Lambda(\nu) & 0\\ 0 & +\Lambda(\mu) & 0 & -\Lambda(\mu) \end{bmatrix},$$

where

$$\Lambda(z)\equiv 2z(1-z)\ .$$

This matrix has eigenvalues

$$\lambda^1=\lambda^2=0,\quad \lambda^3=-2\Lambda(\mu),\quad \lambda^4=-2\Lambda(\nu)\ ,$$

with corresponding left eigenvectors

$$\begin{aligned} &q^1=(+1\ \ 0\ \ +1\ \ 0),\quad q^2=(0\ \ +1\ \ 0\ \ +1)\ ,\\ &q^3=(+1\ \ 0\ \ -1\ \ 0),\quad q^4=(0\ \ +1\ \ 0\ \ -1) \end{aligned} \tag{52}$$

and right eigenvectors

$$q_1=\tfrac{1}{2}\begin{bmatrix}+1\\0\\+1\\0\end{bmatrix},\quad q_2=\tfrac{1}{2}\begin{bmatrix}0\\+1\\0\\+1\end{bmatrix},$$

$$q_3=\tfrac{1}{2}\begin{bmatrix}+1\\0\\-1\\0\end{bmatrix},\quad q_4=\tfrac{1}{2}\begin{bmatrix}0\\+1\\0\\-1\end{bmatrix}.$$

We now construct the Fermi metric. There are two hydrodynamic modes, so $g^{\mu\nu}$ is represented by a 2×2 matrix. From Eq. (22) we see that

$$g^{\mu\nu}=\begin{bmatrix}\Lambda(\mu) & 0\\ 0 & \Lambda(\nu)\end{bmatrix}^{\mu\nu}.$$

The components of the remaining tensors are easily calculated as in the previous examples. The conserved quantities are not ordered, so we can use the results of Sec. III G. The collision operator is not ordered for this lattice gas, so $\mathcal{C}_1^\nu=\mathcal{C}_2^\nu=0$ and there are no advection or source terms in the hydrodynamic equations. The diffusivity is given by Eq. (39),

$$\begin{aligned} \mathcal{D}^\mu{}_\xi&=\frac{c^2}{\Delta t}\left[\sum_{\nu\in K}\frac{\delta(1)^\mu{}_\nu\otimes\mathbf{g}(1)^\nu{}_\xi}{(-\lambda^\nu)}-\frac{1}{2}\mathbf{g}(2)^\mu{}_\xi\right]\\ &=\begin{bmatrix}\mathcal{D}(\nu,\mu)\widehat{\mathbf{x}\mathbf{x}} & 0\\ 0 & \mathcal{D}(\mu,\nu)\widehat{\mathbf{y}\mathbf{y}}\end{bmatrix}^\mu{}_\xi\ , \end{aligned}$$

where we have defined the scalar diffusivities

$$\mathcal{D}(\mu,\nu)\equiv\frac{c^2}{2\Delta t}\left[\frac{2}{(-\lambda^3)}-1\right]=\frac{c^2}{2\Delta t}\left[\frac{1}{2\mu(1-\mu)}-1\right]$$

and

$$\mathcal{D}(\nu,\mu)\equiv\frac{c^2}{2\Delta t}\left[\frac{2}{(-\lambda^4)}-1\right]=\frac{c^2}{2\Delta t}\left[\frac{1}{2\nu(1-\nu)}-1\right]\ .$$

Writing $\nabla=\hat{\mathbf{x}}\partial/\partial x+\hat{\mathbf{y}}\partial/\partial y$, Eq. (37) gives us the pair of hydrodynamic equations

$$\frac{\partial\mu}{\partial t}=\frac{\partial}{\partial x}\left[\mathcal{D}(\nu,\mu)\frac{\partial\mu}{\partial x}\right],\quad \frac{\partial\nu}{\partial t}=\frac{\partial}{\partial y}\left[\mathcal{D}(\mu,\nu)\frac{\partial\nu}{\partial y}\right]\ .$$

Since μ and ν lie in [0,1], it follows that the diffusivities are always positive.

Note that the diffusivity $\mathcal{D}(\mu,\nu)$ of north-south particles depends only on the density μ of east-west particles and vice versa. In the context of the Boltzmann theory, this is because north-south particles scatter only from east-west particles and vice versa. In Sec. VII we compute the effects of correlations on these diffusivities and find that both renormalized diffusivities depend upon both particle densities; this is the reason for including the functional dependence on both densities in $\mathcal{D}$.

D. Lattice-gas fluids

Finally, we consider a class of lattice gases that have been widely used in recent years for the simulation of incompressible Navier-Stokes fluids [1,2]. Such models exist in dimensions two, three, and higher. They conserve mass and momentum, as is appropriate for the Navier-Stokes equations.

The nontrivial collision rules for one of the simplest models of this type, known as the FHP-I model, are shown in Fig. 1. The FHP-I model is defined in two dimensions on a triangular lattice. Note that the two-body collisions have two possible outcomes. We may choose between these by a random bit n^r with mean $\frac{1}{2}$. Variants of this model exist with other three-body and four-body collisions, with rest particles, etc. We use the above model because it is simple but nevertheless fully illustrative for our purposes. Inclusion of the three-body symmetric collision is essential because there would otherwise be three conserved components of momentum.

Consider a general lattice gas with a collision rule preserving particle number and momentum in each direction on a lattice in D dimensions. We assume that bit i at a site represents the presence or absence of a particle of unit mass and momentum $\mathbf{c}^i/\Delta t$. (The restriction to unit mass particles is made only to simplify this presentation and is not in any way essential. Many lattice-gas fluid models allow for particles of different masses.) We can then write the (ensemble-averaged) mass and momentum densities as

$$\rho=\sum_{i=1}^{n} N^i$$

and

$$\mathbf{u}=\sum_{i=1}^{n} \frac{\mathbf{c}^i}{\Delta t} N^i ,$$

respectively. The full set of ensemble-averaged conserved quantities for this problem is thus

$$Q=\begin{bmatrix} \rho \\ \mathbf{u} \end{bmatrix} .$$

Note that this is a $(D+1)$-component column vector since there are D components of conserved momentum density and one conserved mass density. We shall abuse notation by sometimes using ρ and $\mathbf{u}$ as indices; thus we separate the above equation into the components $Q^\rho=\rho$ and $Q^{\mathbf{u}}=\mathbf{u}$. Note that $Q^{\mathbf{u}}$ refers to D distinct components of Q.

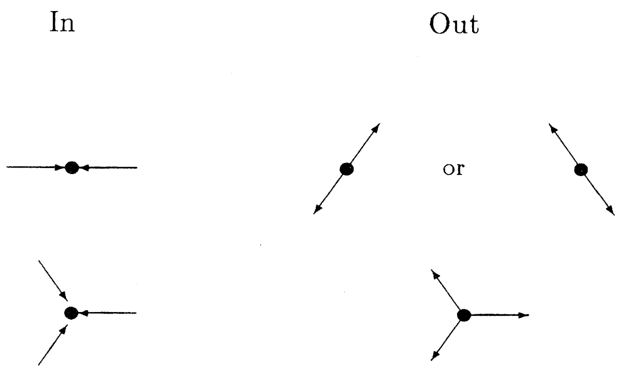


FIG. 1. FHP-I collision rules.

We can at once identify the left hydrodynamic eigenvectors of the system. They are $q_i^\rho=1$ and $q_i^{\mathbf{u}}=\mathbf{c}^i/\Delta t$. To simplify the presentation, we use natural lattice units $(c=\Delta t=1)$ throughout this subsection; we can always reintroduce c and Δt later by dimensional analysis considerations. Thus we write

$$q_i^\rho=1, \quad q_i^{\mathbf{u}}=\mathbf{e}^i .$$

For an incompressible fluid, the conserved densities are ordered in the expansion parameter ϵ as [32]

$$\rho=\rho_0+\epsilon^2\rho_2, \quad \mathbf{u}=\epsilon\mathbf{u}_1 .$$

The second of these equations states that the Mach number is of the same order as the smallness parameter used in the Chapman-Enskog analysis, that is, the Mach number scales as the Knudsen number. The first equation says that the density fluctuations are smaller still; they go as the Mach number squared.

The ordering of the conserved quantities, Eq. (42), for this system is then

$$Q=\begin{bmatrix} \rho \\ \mathbf{u} \end{bmatrix}=\begin{bmatrix} \rho_0 \\ 0 \end{bmatrix}+\epsilon\begin{bmatrix} 0 \\ \mathbf{u}_1 \end{bmatrix}+\epsilon^2\begin{bmatrix} \rho_2 \\ 0 \end{bmatrix}$$
$$=Q_0+\epsilon Q_1+\epsilon^2 Q_2 .$$

Thus the zeroth-order Fermi-Dirac equilibrium is found by considering only q^ρ in Eq. (18). We get

$$N_{00}^i=\frac{1}{1+e^{-\alpha}}\equiv f ,$$

where f is the mean occupation number of the zeroth-order equilibrium. Note that f is strictly constant, independent of spatial position and time.

To proceed, it is necessary to impose some requirements on the lattice. Let us assume that the lattice is a regular lattice and that all tensors formed from outer products of the lattice vectors are isotropic through the fourth rank [22]. That is, we demand that the lattice vectors be such that

$$\sum_{i=1}^{n}\mathbf{e}^i=0, \quad \sum_{i=1}^{n}\mathbf{e}^i\mathbf{e}^i=\frac{n}{D}\mathbf{1} ,$$
$$\sum_{i=1}^{n}\mathbf{e}^i\mathbf{e}^i\mathbf{e}^i=0, \quad \sum_{i=1}^{n}\mathbf{e}^i\mathbf{e}^i\mathbf{e}^i\mathbf{e}^i=\frac{n}{D(D+2)}\mathbf{\Omega} , \tag{53}$$

where we have defined

$$\Omega_{ijkl}=\delta_{ij}\delta_{kl}+\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk} .$$

We can now construct the Fermi metric. There are $D+1$ hydrodynamic modes, so $g^{\mu\nu}$ is a $(D+1)\times(D+1)$ matrix. From Eqs. (22) and (53), we see that it is

$$g^{\mu\nu}=nf(1-f)\begin{bmatrix} 1 & 0 \\ 0 & \frac{1}{D}\mathbf{1} \end{bmatrix}^{\mu\nu} .$$

Since the conserved quantities are ordered, we are going to need the Fermi connection as well. From Eqs. (25) and (53), we see that it is

$$\Gamma^{\eta}{}_{\mu\nu}=-\frac{(1-2f)}{2nf(1-f)}\left[\begin{bmatrix}1&0\\0&D\mathbf{1}\end{bmatrix}_{\mu\nu}\begin{bmatrix}0&1\\1&0\end{bmatrix}_{\mu\nu}\right]^{\eta},$$

where we have used a row of matrices to represent the variation of the three indices; we shall occasionally use this representation for third-rank quantities when it does not cause ambiguity.

Next, we can compute the components of the generalized Fermi metric with hydrodynamic indices. From Eqs. (26) and (27), we have

$$\mathbf{g}(k)^{\mu\nu}=f(1-f)\begin{bmatrix}\sum_i^{k}\otimes\,\mathbf{e}^i & \sum_i^{k+1}\otimes\,\mathbf{e}^i\\ \sum_i^{k+1}\otimes\,\mathbf{e}^i & \sum_i^{k+2}\otimes\,\mathbf{e}^i\end{bmatrix}^{\mu\nu}.$$

Likewise, the components of the generalized Fermi connection are

$$\Gamma(k)^{\eta}{}_{\mu\nu}=-\frac{(1-2f)}{2n^2f(1-f)}$$
$$\times\left[\begin{bmatrix}\sum_i^{k}\otimes\,\mathbf{e}^i & D\sum_i^{k+1}\otimes\,\mathbf{e}^i\\ D\sum_i^{k+1}\otimes\,\mathbf{e}^i & D^2\sum_i^{k+2}\otimes\,\mathbf{e}^i\end{bmatrix}_{\mu\nu}\right.$$
$$\left.\times\begin{bmatrix}\sum_i^{k+1}\otimes\,\mathbf{e}^i & D\sum_i^{k+2}\otimes\,\mathbf{e}^i\\ D\sum_i^{k+2}\otimes\,\mathbf{e}^i & D^2\sum_i^{k+3}\otimes\,\mathbf{e}^i\end{bmatrix}_{\mu\nu}\right]^{\eta}.$$

All of the components of these objects that we shall need can be evaluated from Eqs. (53).

Equation (43) now tells us the form that the hydrodynamic equations will take. We first examine the equation for conservation of mass. Setting the index μ to ρ, we see that the $O(1/\epsilon)$ advection term survives and all the $O(1)$ terms vanish; the next surviving terms are $O(\epsilon)$. Thus, looking to Eq. (45), we get the equation

$$\nabla\cdot\left[\frac{c}{\Delta t}\mathbf{g}(1)^{\rho}{}_{\xi}Q_1^{\xi}\right]=0$$

or, upon simplification,

$$\nabla\cdot\mathbf{u}_1=0\,, \tag{54}$$

to $O(\epsilon^2)$. We recognize this as expressing the condition that the velocity field must have zero divergence in the incompressible limit.

Turning attention next to the equation for conservation of momentum, we set the index μ to $\mathbf{u}$. This time we find that the $O(1/\epsilon)$ part of the advection term vanishes, so the hydrodynamic equation is given by the $O(1)$ terms in Eq. (43). For this situation, Eq. (44) for the advection coefficient reads

$$\begin{aligned}\mathcal{A}^{\mathbf{u}}(\rho_0)=\;&\mathbf{g}(1)^{\mathbf{u}}{}_{\rho}Q_2^{\rho}\\&+[\mathbf{g}(1)^{\mathbf{u}}{}_{\rho}\Gamma^{\rho}{}_{\mathbf{uu}}+\mathbf{g}(1)^{\mathbf{u}}{}_{\mathbf{u}}\cdot\Gamma^{\mathbf{u}}{}_{\mathbf{uu}}\\&-\Gamma(1)^{\mathbf{u}}{}_{\mathbf{uu}}]:\mathbf{u}_1\mathbf{u}_1=P\mathbf{1}+\frac{g(\rho_0)}{\rho_0}\mathbf{u}_1\mathbf{u}_1\,,\end{aligned}$$

where we have defined the factor

$$g(\rho_0)=\frac{D}{D+2}\left[\frac{1-2f}{1-f}\right]$$

and the pressure

$$P\equiv\frac{1}{D}[\rho_2-g(\rho_0)u_1^2] \tag{55}$$

written in lattice units.

Next we turn our attention to the diffusivity tensor $\mathcal{D}^{\mathbf{u}}{}_{\mathbf{u}}$, given by Eq. (39). We have

$$\delta(1)^{\mathbf{u}}{}_{\nu}=q_j^{\mathbf{u}}\mathbf{e}^jq_{\nu}^j=\sum_{j=1}^{n}q_{\nu}^j\mathbf{e}^j\mathbf{e}^j\,,$$

$$\mathbf{g}(1)^{\nu}{}_{\mathbf{u}}=g_{\mathbf{uu}}\mathbf{g}(1)^{\mathbf{u}\nu}=\frac{D}{n}\sum_{j=1}^{n}q_j^{\nu}\mathbf{e}^j\mathbf{e}^j\,,$$

$$\mathbf{g}(2)^{\mathbf{u}}{}_{\mathbf{u}}=g_{\mathbf{uu}}\mathbf{g}(2)^{\mathbf{uu}}=\frac{D}{n}\sum_{j=1}^{n}\mathbf{e}^j\mathbf{e}^j\mathbf{e}^j\mathbf{e}^j=\frac{1}{D+2}\mathbf{\Omega}\,,$$

so Eq. (39) becomes

$$(\mathcal{D}^{u_i}{}_{u_l})^j_k=\frac{c^2}{(D+2)\Delta t}\left\{\frac{D(D+2)}{n}\mathbf{e}_i^m\mathbf{e}_j^m\mathbf{e}_k^p\mathbf{e}_l^p\right.$$
$$\left.\times\left[\sum_{\nu\in K}\frac{q_{\nu}^mq_p^{\nu}}{(-\lambda^{\nu})}\right]-\frac{1}{2}\mathbf{\Omega}_{ijkl}\right\}, \tag{56}$$

where we have made it clear that $\mathcal{D}^{\mathbf{u}}{}_{\mathbf{u}}$ is a fourth-rank object by explicitly writing the four spatial indices i, j, k, and l and where there is an implicit sum over m and p. Now since the principal fourth-rank tensor constructed from our lattice vectors [see Eq. (53)] is isotropic and since we have done nothing else to break isotropy, this fourth-rank tensor must be isotropic as well. That means that it must be of the form

$$(\mathcal{D}^{u_i}{}_{u_l})^j_k=\nu\delta_{il}\delta_{jk}+\alpha\delta_{ij}\delta_{lk}+\beta\delta_{ik}\delta_{lj}\,, \tag{57}$$

so that the diffusive term on the right-hand side of the hydrodynamic equation becomes

$$\nabla_j(\mathcal{D}^{u_i}{}_{u_l})^j_k\nabla_ku_l=\nu\nabla^2u_i+\nabla_i[(\alpha+\beta)\nabla\cdot\mathbf{u}]\,.$$

Note that the second term on the right-hand side vanishes due to the incompressibility condition, Eq. (54), and ν emerges as the shear viscosity in the hydrodynamic equation (43), which can now be written

$$\frac{\partial\mathbf{u}_1}{\partial t}+\frac{g(\rho_0)}{\rho_0}\mathbf{u}_1\cdot\nabla\mathbf{u}_1=-\nabla P+\nu\nabla^2\mathbf{u}\,. \tag{58}$$

With the exception of the pathological factor $g(\rho_0)$ in the inertial term, which we shall address below, we recognize this as the incompressible Navier-Stokes equation. (Recall that **u** is the momentum density, not the hydrodynamic velocity.)

To get a closed expression for the viscosity ν, we take the following traces of Eq. (57):

$$(\mathcal{D}^{u_i}{}_{u_i})^j_j = D\alpha + D\beta + D^2\nu ,$$

$$(\mathcal{D}^{u_i}{}_{u_j})^j_i = D\alpha + D^2\beta + D\nu ,$$

$$(\mathcal{D}^{u_i}{}_{u_j})^i_j = D^2\alpha + D\beta + D\nu .$$

These three equations may be solved for ν to yield

$$\nu = \frac{(D+1)(\mathcal{D}^{u_i}{}_{u_i})^j_j - (\mathcal{D}^{u_i}{}_{u_j})^j_i - (\mathcal{D}^{u_i}{}_{u_j})^i_j}{D(D-1)(D+2)} .$$

Inserting Eq. (56), after a bit of algebra we get the following result for the viscosity of a lattice fluid:

$$\nu = \frac{c^2}{(D+2)\Delta t}\left[\frac{D}{n(D-1)}\sum_{\nu\in K}\frac{q^m_\nu(\mathbf{e}^m\cdot\mathbf{e}^n)^2 q^\nu_n}{(-\lambda^\nu)} - \frac{1}{2}\right] . \tag{59}$$

We can compare this result with that of Hénon [22],

$$\nu = \frac{c^2}{(D+2)\Delta t}\left[\lambda_H - \frac{1}{2}\right] ,$$

where the quantity λ_H is given by

$$\frac{1}{\lambda_H} \equiv \frac{1}{2n}\left[\frac{D}{D-1}\right]\sum_{s,s'} A(s\to s')f^{p-1}(1-f)^{n-p-1} \times[\mathbf{Y}(s)-\mathbf{Y}(s')]:[\mathbf{Y}(s)-\mathbf{Y}(s')] ,$$

where $\mathbf{Y}(s)$ is the traceless part of $\mathbf{X}(s)$

$$\mathbf{Y}(s) \equiv \mathbf{X}(s) - \frac{p}{D}\mathbf{1}$$

and $\mathbf{X}(s)$ is in turn given by

$$\mathbf{X}(s) \equiv \sum_j s^j \mathbf{e}^j \mathbf{e}^j$$

with trace

$$p \equiv \mathrm{Tr}[\mathbf{X}(s)] = \sum_j s^j .$$

Note that our analysis has yielded an alternative expression for Hénon's quantity,

$$\lambda_H = \frac{1}{n}\left[\frac{D}{D-1}\right]\sum_{\nu\in K}\frac{q^m_\nu(\mathbf{e}^m\cdot\mathbf{e}^n)^2 q^\nu_n}{(-\lambda^\nu)} .$$

So far, we have assumed only that the lattice vectors satisfy Eqs. (53) and that the particles have unit mass and speed. To evaluate Eq. (59) for the shear viscosity, however, it is necessary to specify a particular collision rule.

Thus we now specialize to the FHP-I lattice gas, in two dimensions ($D=2$), with six bits per site ($n=6$), and with lattice vectors given by

$$\mathbf{e}^j = \cos\left[\frac{2\pi j}{6}\right]\hat{\mathbf{x}} + \sin\left[\frac{2\pi j}{6}\right]\hat{\mathbf{y}} .$$

We then have

$$(\mathbf{e}^j\cdot\mathbf{e}^k)^2 = \cos^2\left[\frac{2\pi(j-k)}{6}\right] = \begin{bmatrix} 1 & \frac14 & \frac14 & 1 & \frac14 & \frac14 \\ \frac14 & 1 & \frac14 & \frac14 & 1 & \frac14 \\ \frac14 & \frac14 & 1 & \frac14 & \frac14 & 1 \\ 1 & \frac14 & \frac14 & 1 & \frac14 & \frac14 \\ \frac14 & 1 & \frac14 & \frac14 & 1 & \frac14 \\ \frac14 & \frac14 & 1 & \frac14 & \frac14 & 1 \end{bmatrix}^{jk} .$$

The collision rules are illustrated in Fig. 1. We form the Jacobian of the collision operator from Eq. (30). Because the collision rules are invariant under cyclic interchange of the lattice vectors, the Jacobian is a circulant matrix, so it is particularly easy to write down its eigenvalues and eigenvectors [21]. We find

$$\lambda^1 = \lambda^2 = \lambda^3 = 0 ,$$

$$\lambda^4 = \lambda^6 = -3f(1-f)^3 ,$$

$$\lambda^5 = -6f^2(1-f)^2 ,$$

with corresponding left eigenvectors

$$q_1 = (+1 \ \ +1 \ \ +1 \ \ +1 \ \ +1 \ \ +1) ,$$

$$q_2 = \frac{\sqrt{3}}{2}(0 \ \ +1 \ \ +1 \ \ 0 \ \ -1 \ \ -1) ,$$

$$q_3 = \frac{1}{2}(+2 \ \ +1 \ \ -1 \ \ -2 \ \ -1 \ \ +1) ,$$

$$q_4 = \frac{1}{2}(+2 \ \ -1 \ \ -1 \ \ +2 \ \ -1 \ \ -1) ,$$

$$q_5 = (+1 \ \ -1 \ \ +1 \ \ -1 \ \ +1 \ \ -1) ,$$

$$q_6 = \frac{\sqrt{3}}{2}(0 \ \ +1 \ \ -1 \ \ 0 \ \ +1 \ \ -1)$$

and right eigenvectors

$$q^1 = \tfrac16\begin{bmatrix}+1\\+1\\+1\\+1\\+1\\+1\end{bmatrix} ,\quad q^2 = \frac{\sqrt{3}}{6}\begin{bmatrix}0\\+1\\+1\\0\\-1\\-1\end{bmatrix} ,\quad q^3 = \tfrac16\begin{bmatrix}+2\\+1\\-1\\-2\\-1\\+1\end{bmatrix} ,$$

$$q^4 = \tfrac16\begin{bmatrix}+2\\-1\\-1\\+2\\-1\\-1\end{bmatrix} ,\quad q^5 = \tfrac16\begin{bmatrix}+1\\-1\\+1\\-1\\+1\\-1\end{bmatrix} ,\quad q^6 = \frac{\sqrt{3}}{6}\begin{bmatrix}0\\+1\\-1\\0\\+1\\-1\end{bmatrix} .$$

It is now a simple matter to plug these quantities into Eq. (59) to obtain the shear viscosity (we now restore the dimensioned quantities c and Δt)

$$\nu = \frac{c^2}{8\Delta t}\left[\frac{1}{(-\lambda^4)} + \frac{1}{(-\lambda^6)} - 1\right] = \frac{c^2}{\Delta t}\left[\frac{1}{12f(1-f)^3} - \frac{1}{8}\right] ,$$

which is the expected result for the viscosity of the FHP-I lattice gas under the Boltzmann approximation [2,21].

To conclude this subsection, we discuss the pathological factor $g(\rho_0)$ that appears in front of the inertial term of the Navier-Stokes equation (58). Note that the convective derivative operator $\partial_t + \mathbf{u}\cdot\nabla$ is Galilean invariant since it retains its form under a Galilean transformation $\mathbf{x} \to \mathbf{x}' + \mathbf{V}t'$ and $t \to t'$. Thus the presence of the $g(\rho_0)$ factor in the inertial term is reflective of a breakdown of Galilean invariance. As has been pointed out by numerous authors [1,2,21], this is not surprising since the lattice itself constitutes a preferred Galilean frame of reference.

In practical simulations of incompressible fluids, this factor is not a problem since it is constant and can be removed by a simple rescaling of either the dependent or independent variables. Similarly, the rather unphysical equation of state (55) is not a problem since the equation of state is irrelevant in the incompressible limit. Efforts to extend lattice-gas methods to treat compressible fluids, however, must deal with these problems. Techniques are known for doing this, but they are outside the scope of this paper.

V. EXAMPLE CALCULATION

In this section we give a simple example of how correlations between particles in the 1D3P lattice gas give rise to a modification of the Boltzmann equation. This example calculation is intended to serve as an introduction to the more general analysis of the following section. The reader may thus find it useful to refer back to this example while working through the following sections.

In the 1D3P lattice gas, the dynamical variables are the bits $n^i(x,t)$, where $i \in \{-,0,+\}$ and x and t are integer-valued space and time coordinates. We shall choose a particular variable $n^+(3,3)$ and describe some of the corrections to the Boltzmann equation for this variable.

If we take the ensemble average of the collision operator Eq. (47), we can write an exact equation for the density of the bit we are interested in:

$$\begin{aligned} N^0(3,3) = N^0(3,2) &+ 2p\langle n^+(2,2)n^-(4,2)\rangle \\ &- p\langle n^0(3,2)n^+(2,2)\rangle \\ &- p\langle n^-(4,2)n^0(3,2)\rangle \ . \end{aligned} \tag{60}$$

Figure 2 depicts in a graphical form the set of variables that appears in this equation. (Throughout, we shall depict diagrams for one-dimensional lattice gases with a vertical time axis.) Applying the Boltzmann approximation to Eq. (60) would reproduce the Boltzmann equation as stated in Sec. IV A. This approximation is corrected by the existence of correlations between the pairs of variables in the two-particle means. The two-particle connected correlation function is defined to be the difference between the mean of a product and the product of the means (we denote single-particle means by capital letters as usual),

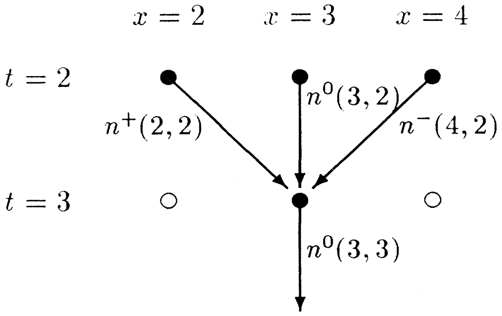


FIG. 2. Diagram of variables appearing in the equation for $N^+(3,3)$.

$$\Gamma(x,y) = \langle xy\rangle - XY \ .$$

Thus the correction to the Boltzmann approximation for Eq. (60) is given by

$$\begin{aligned} \delta N^0(3,3) = {} & 2p\Gamma(n^+(2,2),n^-(4,2)) \\ & - p\Gamma(n^0(3,2),n^+(2,2)) \\ & - p\Gamma(n^-(4,2),n^0(3,2)) \ . \end{aligned} \tag{61}$$

We have now expressed the mean of a particular variable in terms of the means and connected correlation functions of the variables at the previous time step. In order to analyze the exact equations of motion for a lattice gas, we are interested in constructing an equation where the expression on the right-hand side is given completely in terms of single-particle means. To accomplish this, we must express the correlation functions in Eq. (61) in terms of means at still earlier time steps. As an example, we consider the term

$$\Gamma(n^0(3,2),n^+(2,2)) \ .$$

This term appears with a coefficient of $-p$ in Eq. (61); such a coefficient will be called a *correlation vertex coefficient* in Sec. VI. To calculate this correlation function in terms of the means and correlation functions at time $t=1$, we can use the equation of motion for each of the two bits in turn. We have

$$\begin{aligned} \Gamma(n^0(3,2),n^+(2,2)) &= \langle n^0(3,2)n^+(2,2)\rangle - \langle n^0(3,2)\rangle\langle n^+(2,2)\rangle \\ &= \Gamma(n^0(3,2),n^+(1,1)) + 2p\Gamma(n^0(3,2),n^0(2,1),n^-(3,1)) \\ &\quad + 2pN^-(3,1)\Gamma(n^0(3,2),n^0(2,1)) + 2pN^0(2,1)\Gamma(n^0(3,2),n^-(3,1)) \\ &\quad - p\Gamma(n^0(3,2),n^+(1,1),n^-(3,1)) - pN^-(3,1)\Gamma(n^0(3,2),n^+(1,1)) \\ &\quad - pN^+(1,1)\Gamma(n^0(3,2),n^-(3,1)) - p\Gamma(n^0(3,2),n^0(2,1),n^+(1,1)) \\ &\quad - pN^+(1,1)\Gamma(n^0(3,2),n^0(2,1)) - pN^0(2,1)\Gamma(n^0(3,2),n^+(1,1)) \ , \end{aligned}$$

where we have expanded three-particle means in terms of connected correlation functions using the cluster expansion

$$\langle xyz\rangle=\Gamma(x,y,z)+Z\Gamma(x,y)+Y\Gamma(x,z)+X\Gamma(z,y)+XYZ\ .$$

We select a single term

$$\Gamma(n^0(3,2),n^-(3,1))$$

for further analysis. This term appears in the above expression with a coefficient of $2pN^0(2,1)-pN^+(1,1)$. As we shall discuss in Sec. VI, when we are performing the Chapman-Enskog analysis around a homogeneous equilibrium, connected correlations in a semidetailed balance lattice gas are always of order ϵ. Thus, in an order ϵ analysis, we can substitute the equilibrium values for the single-particle means, giving us a coefficient of pf. Using the same argument as above,

$$\begin{aligned}\Gamma(n^-(3,1),n^0(3,2))&=\langle n^-(3,1)n^0(3,2)\rangle-\langle n^-(3,1)\rangle\langle n^0(3,2)\rangle\\&=\Gamma(n^-(3,1),n^0(3,1))+2p\Gamma(n^-(3,1),n^+(2,1),n^-(4,1))\\&\quad+2pN^-(4,1)\Gamma(n^-(3,1),n^+(2,1))+2pN^+(2,1)\Gamma(n^-(3,1),n^-(4,1))\\&\quad-p\Gamma(n^-(3,1),n^0(3,1),n^-(4,1))-pN^-(4,1)\Gamma(n^-(3,1),n^0(3,1))\\&\quad-pN^0(3,1)\Gamma(n^-(3,1),n^-(4,1))-p\Gamma(n^-(3,1),n^+(2,1),n^0(3,1))\\&\quad-pN^0(3,1)\Gamma(n^-(3,1),n^+(2,1))-pN^+(2,1)\Gamma(n^-(3,1),n^0(3,1))\ .\end{aligned}$$

Once again, we shall analyze only a subset of these terms. We extract the coefficient of

$$\Gamma(n^-(3,1),n^0(3,1))\ ,$$

which is (inserting the equilibrium values)

$$1-pN^-(4,1)-pN^+(2,1)=1-2pf+O(\epsilon^2)\ .$$

Let us recapitulate the analysis so far. We have written the exact equation for the variable $n^+(3,3)$ in terms of means and connected correlation functions at earlier time steps. We have continued to expand the correlation functions in terms of earlier time steps and have concluded that theer is a plethora of corrections to the Boltzmann equation, included in which is the term

$$\begin{aligned}\delta N^0(3,3)=\cdots&+(-p)(pf)(1-2pf)\\&\times\Gamma(n^-(3,1),n^0(3,1))+\cdots\ .\end{aligned}\tag{62}$$

We now wish to continue the process one step further by expressing this correlation function in terms of the means and correlations at time $t=0$. Because the correlated variables are at the same vertex ($x=3$), we cannot expand the equations of motion for the variables separately. Instead, we must use the state transition table from Sec. IV A to directly compute the two-particle mean

$$\begin{aligned}\langle n^-(3,1)n^0(3,1)\rangle=&(1-2p)\langle n^-(4,0)n^0(3,0)\rangle\\&+p\langle n^-(4,0)n^+(2,0)\rangle\\&+p\langle n^+(2,0)n^0(3,0)\rangle\ .\end{aligned}\tag{63}$$

We can now combine Eq. (63) with the exact equations for the single-particle means of $n^-(3,1)$ and $n^0(3,1)$ to compute the correlation function from Eq. (62). We are particularly interested in the terms that contain only single-particle means since these terms will directly modify the original Boltzmann equation without having to further expand connected correlation functions. Thus, neglecting correlations on the right-hand side we have

$$\begin{aligned}\Gamma(n^-(3,1),n^0(3,1))=&(1-2p)N^-(4,0)N^0(3,0)+pN^-(4,0)N^+(2,0)+pN^+(2,0)N^0(3,0)\\&-[N^-(4,0)+2pN^0(3,0)N^+(2,0)-pN^-(4,0)N^0(3,0)-pN^-(4,0)N^+(2,0)]\\&\times[N^0(3,0)+2pN^-(4,0)N^+(2,0)-pN^-(4,0)N^0(3,0)-pN^0(3,0)N^+(2,0)]\ .\end{aligned}$$

As in the Boltzmann–Chapman-Enskog analysis, we assume that the deviations of the single-particle means from equilibrium are of order ϵ, so we can take derivatives and get

$$\begin{aligned}\Gamma(n^-(3,1),n^0(3,1))=&-pf(1-f)N_1^-(4,0)\\&-pf(1-f)N_1^0(3,0)\\&+2pf(1-f)N_1^+(2,0)+O(\epsilon^2)\ .\end{aligned}\tag{64}$$

Combining this with Eq. (62), we have calculated a set of terms that appears in the exact equations of motion of the 1D3P lattice gas. By carrying out such a calculation for every correlation function appearing in the expansion of Eq. (61), we could write the exact lattice-gas equation as an infinite sum of such terms. It might seem that summing this infinite series of terms and accounting for their effects on the dynamics of a lattice gas is a hopeless task. However, for many lattice gases it turns out that the only effect of this infinite series of terms is to modify (renormalize) the eigenvalues of the Jacobian matrix by a finite amount.

For example, if we combine Eqs. (62) and (64), we see that

$$\frac{\partial N^0(3,3)}{\partial N_1^0(3,0)} = \cdots - pf(1-f)(-p)(pf)(1-2pf) + \cdots .$$

Noting that $N_1^*(x,0)$ differs from $N_1^*(x,3)$ only by $O(\epsilon^2)$, we see that this is a correction to the Jacobian element $J^0{}_0$ of Eq. (49). Moreover, the paths of the correlated quantities that gave rise to this term can be illustrated by the graph in Fig. 3. The fact that the initial and final arrows are in the 0 direction indicates that this is a correction to $J^0{}_0$, and we note that the factors in this correction can be associated with the vertices of this graph, as shown.

In the following section we develop a systematic approach for computing the correction terms in the exact lattice-gas equations. We develop a diagrammatic method for categorizing the correction terms and demonstrate that the diagrams can be grouped into sets, whose combined effects on the dynamics are simply to renormalize the eigenvalues of the Jacobian matrix.

VI. EXACT ANALYSIS

We now proceed to develop in a more general context the exact description of hydrodynamic behavior in the scaling limit, dropping the molecular chaos assumption and including effects due to correlations. As mentioned in Sec. I, the diagrammatic formalism we develop here is similar in many ways to the analogous formalism for continuum kinetic theory. Unlike continuous systems, however, the discrete nature of lattice gases allows us to explicitly write the complete set of terms that contributes correlations over a finite time interval as a sum over a finite number of diagrams. The discretization of lattice gases also changes the nature of the vertices in correlation diagrams. In a lattice-gas system, the vertices represent correlation interactions at a single lattice site and can be simply calculated from the time-development equation. There is a finite number of distinct vertex types, corresponding to correlated particles arriving at and departing from a single lattice point at a single time step.

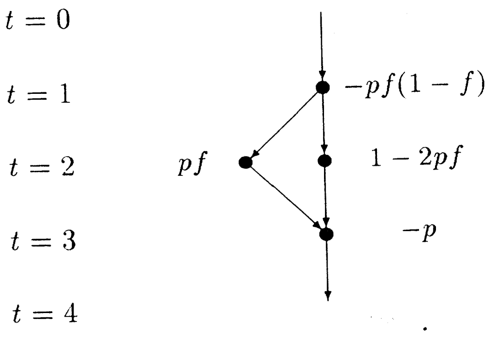


FIG. 3. Example diagram correcting the Jacobian for the 1D3P model.

In Sec. VI A we generalize our notation slightly to deal with arbitrary sets of particles on the lattice. We begin developing the diagrammatic formalism for lattice gases in Sec. VI B by discussing several alternate descriptions of correlations in ensembles. In Sec. VI C we express a renormalized version of the Jacobian matrix $J^i{}_j$ in terms of an infinite series. The terms in this series are factorized into independent contributions from each lattice site in Sec. VI D and written in diagrammatic notation in Sec. VI E. In Sec. VI F we describe how several useful approximations, such as the ring approximation, can be calculated in our formalism as a sum over a restricted class of diagrams. In Sec. VI G, we prove that a fairly wide class of lattice gases has the property that the only effect of correlations is to modify the eigenvalues of the J matrix in terms of which the transport coefficients are described. Finally, in Sec. VI H, we describe the effects of the higher-order collision terms Ω_1^i and Ω_2^i on the exact hydrodynamic equations.

In Secs. VII and VIII we apply the techniques of this section to the lattice gases described in Sec. IV. The reader may find it helpful to refer to Secs. V, VII, and VIII for concrete examples of the formalism while reading this section.

A. General notation

In this subsection, we develop a slightly more general system of notation suitable for describing the exact dynamics of a lattice gas. This notation is similar to the matrix form of notation used in Sec. II; however, we now wish to consider the space of all configurations of the full system rather than simply the set of states at a single lattice point.

Recall that we can refer to an arbitrary bit of the system by an index $a \in \mathcal{B}$. We now introduce a *propagation operator* $\mathcal{P}^b{}_c$, which acts on the space of bits in the entire system. This operator is an $N \times N$ permutation matrix. It connects bit b with bit c if and only if the particle represented by bit c moves into bit b during the propagation substep, that is,

$$\mathcal{P}^b{}_c = \begin{cases} 1 & \text{if } b = a(i(c), \mathbf{x}(c) + \mathbf{c}^{i(c)}) \\ 0 & \text{otherwise} . \end{cases}$$

In terms of this operator, the exact dynamical equation for the lattice gas (1) may be written

$$n^b(t+\Delta t) = \mathcal{P}^b{}_c(n^c(t) + \omega^{i(c)}(n^{a(*,\mathbf{x}(c))}(t))) \tag{65}$$

and the lattice Boltzmann equation (11) may be written

$$N^b(t+\Delta t) = \mathcal{P}^b{}_c(N^c(t) + \Omega^{i(c)}(N^{a(*,\mathbf{x}(c))}(t))) . \tag{66}$$

We denote the ensemble mean of an arbitrary product of the n^a's by

$$N^\alpha = \left\langle \prod_{a \in \alpha} n^a \right\rangle , \quad \alpha \subseteq \mathcal{B} .$$

Henceforth, we use the greek letters $\alpha, \beta, \ldots$ to denote subsets of the set $\mathcal{B}$ and the letters $\mu, \nu, \ldots$ to denote subsets of B. We shall sometimes use a latin index to denote an index set with a single element, as in $N^a = N^{\{a\}}$. Additionally, for quantities subscripted or superscripted by a single set, we shall sometimes replace the set by its elements, as in $N^{abc} = N^{\{a,b,c\}}$. As a final point of notation, an index set with a circumflex is assumed to have at least two elements, i.e., $|\hat{\alpha}| \geq 2$.

Finally, we generalize the propagation operator $\mathcal{P}$ to be a permutation matrix $\mathcal{P}^{\alpha}{}_{\beta}$ acting on the 2^N-dimensional space of subsets of $\mathcal{B}$. For a fixed set of bits $\beta = \{b_1, \ldots, b_q\} \subseteq \mathcal{B}$, if we take $\alpha = \{a_1, \ldots, a_q\}$ to be the set of particles which β goes to under propagation, i.e., $a_j = a(i(b_j), \mathbf{x}(b_j) + \mathbf{c}^{i(b_j)})$, then

$$\mathcal{P}^{\alpha'}{}_{\beta} = \begin{cases} 1, & \alpha' = \alpha \\ 0, & \alpha' \neq \alpha \ . \end{cases}$$

Thus, for example, $\mathcal{P}^{a}{}_{b}$ is 1 when $a = a(i(b), \mathbf{x}(b) + \mathbf{c}^{i(b)})$ and 0 otherwise, in agreement with the previous notation.

B. Representations of correlations

An ensemble is generally defined to be a distribution on the space of possible configurations of the entire lattice-gas system. In this subsection, we discuss several alternative descriptions of the probability distribution describing an ensemble.

Given a set S of Boolean variables $S = \{n^1, n^2, \ldots, n^N\}$, a probability distribution on S can be described in several equivalent ways. The most familiar description is given by assigning a probability to each possible set of values for the n^{α}'s, i.e., given any set $\alpha \subseteq \{1, 2, \ldots, N\}$, we define the probability that the corresponding set of n's is equal to 1 and the rest are 0 to be

$$P^{\alpha} = [\text{probability that } (n^1, n^2, \ldots, n^N) = (\chi^{\alpha}(1), \chi^{\alpha}(2), \ldots, \chi^{\alpha}(N))] \ ,$$

where

$$\chi^{\alpha}(i) = \begin{cases} 1, & i \in \alpha \\ 0, & i \notin \alpha \ . \end{cases}$$

Since there are 2^N such subsets α and since

$$\sum_{\alpha} P^{\alpha} = 1$$

is the only constraint, the space of probability distributions on these N variables is $(2^N - 1)$ dimensional. [In fact, it is a $(2^N - 1)$-dimensional simplex.]

An equivalent description of a probability distribution on S can be given by defining the means N^{α} for each possible product of elements of S. [Note that $(n^a)^2 = n^a$, so that the mean of any product of elements of S is equal to N^{α} for some α.]

In terms of the P^{α}'s, the means can be expressed as

$$N^{\alpha} = \sum_{\beta \supseteq \alpha} P^{\beta} \ . \tag{67}$$

This relationship can be inverted to get

$$P^{\alpha} = \sum_{\beta \supseteq \alpha} (-1)^{|\beta| - |\alpha|} N^{\beta} \ . \tag{68}$$

The space of allowed values for the means is also $2^N - 1$ dimensional since $N^{\varnothing} = 1$. These two descriptions of a distribution are equivalent in the sense that the information contained in either description is exactly sufficient to completely specify the distribution. In fact, Eqs. (67) and (68) show that the probabilities and the multipoint means are related by a linear transformation.

Probability distributions in which the n^a are distributed independently have means given by

$$N^{\alpha} = \prod_{a \in \alpha} N^a \ .$$

The space of *independent* distributions on N variables is clearly N dimensional and is parametrized by N^a, $a \in \{1, 2, \ldots, N\}$. The Fermi-Dirac equilibrium (18) is an example of an independent distribution.

A third description of a distribution on S can be given in terms of *connected correlation functions* (CCF's) [33]. An expansion in CCF's is often referred to as a *cluster expansion*. For each $\alpha \subseteq \{1, 2, \ldots, N\}$, there is a CCF, which we denote by Γ^{α}. It is easiest to define the CCF's implicitly by expressing the means in terms of the CCF's through the equation

$$N^{\alpha} = f^{\alpha}(\Gamma^*) = \sum_{\zeta \in \pi(\alpha)} \Gamma^{\zeta_1} \Gamma^{\zeta_2} \cdots \Gamma^{\zeta_q} \ , \tag{69}$$

where $\pi(\alpha)$ is the set of all partitions of α into disjoint subsets $\zeta_1, \ldots, \zeta_q$. Explicitly,

$$\begin{aligned} N^a &= \Gamma^a \ , \\ N^{ab} &= \Gamma^{ab} + \Gamma^a \Gamma^b \ , \\ N^{abc} &= \Gamma^{abc} + \Gamma^a \Gamma^{bc} + \Gamma^b \Gamma^{ac} + \Gamma^c \Gamma^{ab} + \Gamma^a \Gamma^b \Gamma^c \ , \\ &\vdots \ . \end{aligned}$$

We shall refer to N^{α} (Γ^{α}) as an n-mean (n-CCF), when $|\alpha| = n$. The above set of equations can be inverted by induction on n to get a functional relationship of the form

$$\Gamma^{\alpha} = g^{\alpha}(N^*) \ , \tag{70}$$

where g and f are inverses. Explicitly, we have

$$\begin{aligned} \Gamma^a &= N^a \ , \\ \Gamma^{ab} &= N^{ab} - N^a N^b \ , \\ \Gamma^{abc} &= N^{abc} - N^a N^{bc} - N^b N^{ac} - N^c N^{ab} + 2 N^a N^b N^c \ , \\ &\vdots \ . \end{aligned}$$

Again, the description of a probability distribution in terms of CCF's is completely equivalent to the descriptions in terms of N^{α}'s and P^{α}'s. There are $2^N - 1$ independent Γ^{α}'s, as $\Gamma^{\varnothing}$ is not defined. Note that the relationship between the Γ^{α}'s and the N^{α}'s (or the P^{α}'s) is nonlinear.

The main reason that CCF's will be a useful description for us is that in a Gibbsian equilibrium all n-CCF's are 0, for $n > 1$. Thus the distance of a distribution from one that is independent is measured by the quantities $\Gamma^{\hat{\alpha}}$ (recall that an index set with a circumflex is constrained to have more than one element). In the subsequent analysis, we shall find both the N^{α} and Γ^{α} notations to be useful and we shall use the functions f and g to move between the two descriptions.

C. Exact dynamics

We now proceed to rewrite the exact dynamical equation for the lattice gas (65) in a form similar to that of the lattice Boltzmann equation. For most of this section we shall assume that the collision operator respects the conservation laws exactly and obeys semidetailed balance, so that $\omega^i=\omega_0^i$ and $\omega_1^i=\omega_2^i=0$; in Sec. VI H we shall discuss the effect of correlations when we include nonzero ω_1^i and ω_2^i.

Recall that the collision operator in the lattice Boltzmann equation (66) can be linearized, as in Eq. (29), to give

$$N^b(t+\Delta t)=\mathcal{P}^b{}_c(N^c(t)+\epsilon J^{i(c)}{}_j N_1^{a(j,\mathbf{x}(c))}(t)) \ . \tag{71}$$

In order to describe the macroscopic behavior of the system we need only include the effect of the collision operator Ω_0^i up to the order ϵ term associated with the Jacobian since, as we have seen in Sec. III, the higher-order terms associated with the collision operator have no effect upon the hydrodynamic equations of the system. In fact, the hydrodynamic equations derived in Sec. III, and the associated advective and diffusive transport coefficients, depend upon only the Jacobian matrix $J^i{}_j$, through its eigenvalues and eigenvectors. What we now wish to show is that if we drop the Boltzmann molecular chaos assumption and analyze the exact ensemble-averaged equation of motion for a lattice gas in the scaling limit, we get an equation identical in form to Eq. (71), but with a *renormalized* J matrix. The exact transport coefficients can then be expressed in terms of the eigenvalues and eigenvectors of the renormalized J matrix using precisely the same expressions as in the Boltzmann analysis. Furthermore, we find that for a large class of lattice gases, the eigenvectors of the renormalized J matrix are unchanged; only the eigenvalues of the matrix undergo renormalization due to correlations.

We begin with the exact time-development equation (65). By taking the ensemble average of the product of this equation over all a in an arbitrary set $\alpha\subseteq\mathcal{B}$, we can write the exact equation for an arbitrary multipoint mean at time $t+\Delta t$ in terms of multipoint means at time t. We have

$$\begin{aligned} N^{\alpha}(t+\Delta t) &= \left\langle \prod_{a\in\alpha} n^a(t+\Delta t)\right\rangle \\ &= \sum_{\beta} \mathcal{P}^{\alpha}{}_{\beta}\left\langle \prod_{b\in\beta} [n^b(t)+\omega^{i(b)}(n^*(\mathbf{x}(b),t))]\right\rangle \ . \end{aligned} \tag{72}$$

To express the right-hand side in terms of multipoint means, it will be convenient to rewrite this equation in a more compact notation. For a set $\beta\subseteq\mathcal{B}$, let us define L_β to be the subset of points in L that contain at least one particle in the set β, that is,

$$L_\beta=\{\mathbf{y}\in L\colon \mathbf{x}(b)=\mathbf{y} \ \text{ for some } b\in\beta\} \ .$$

Similarly, we define $\beta_{\mathbf{x}}$ to be the set of i's corresponding to the particles in β at the point $\mathbf{x}$, that is,

$$\beta_{\mathbf{x}}=\{i\in B\colon a(i,\mathbf{x})\in\beta\} \ .$$

We can now factorize the product appearing on the right-hand side of Eq. (72) into contributions from each of the points in L_β by writing

$$\prod_{b\in\beta}[n^b(t)+\omega^{i(b)}(n^*(\mathbf{x}(b),t))] = \prod_{\mathbf{x}\in L_\beta}\prod_{i\in\beta_{\mathbf{x}}}[n^i(\mathbf{x},t)+\omega^i(n^*(\mathbf{x},t))] \ .$$

The innermost product on the right now depends only on quantities at a single site $\mathbf{x}$.

The functions $\omega^i(n^*)$ can be expressed as polynomials in the n^i's of the form

$$\omega^i(n^*)=\sum_{\nu\subseteq B} k^i{}_\nu \prod_{j\in\nu} n^j \ ,$$

where the $k^i{}_\nu$ are coefficients that may depend only on random bits at each lattice site and are constant for deterministic lattice gases. Thus we can write

$$\prod_{i\in\mu}[n^i+\omega^i(n^*)]=v^{\mu}{}_{\nu}\prod_{j\in\nu} n^j \ ,$$

where the quantities $v^{\mu}{}_{\nu}$ may contain random bits at each site. Taking the ensemble average over any such random bits, we get the *mean vertex coefficients* $V^{\mu}{}_{\nu}$

$$V^{\mu}{}_{\nu}=\langle v^{\mu}{}_{\nu}\rangle \ . \tag{73}$$

The state transition probabilities $A(s\to s')$ may be interpreted as elements of a collision matrix on the space of probabilities P^s in the sense that the postcollision probability of a state s' is given by

$$\sum_s A(s\to s')P^s \ . \tag{74}$$

Similarly, the matrix $V^{\mu}{}_{\nu}$ can be interpreted as a collision matrix on the space of means. Using Eqs. (67), (68), and (74), the matrix V can be related to A through the equation

$$V^{\mu}{}_{\nu}=\sum_{s'\supseteq\mu}\sum_{s\subseteq\nu}(-1)^{|\nu|-|s|}A(s\to s') \ , \tag{75}$$

where we have identified the state s with the set of bits that are 1 in that state ($s\subseteq B$). Referring back to the example calculation of Sec. V, observe that the coefficients in Eq. (63) are precisely the mean vertex coefficients for the 1D3P lattice gas. Clearly, the 2^{2n} matrix elements $V^{\mu}{}_{\nu}$ depend only on the sets μ and ν and on the form of the collision operator. In particular, they do not depend on $\mathbf{x}$ or on the values of the n^a's. Note that $V^{\varnothing}{}_{\nu}=\delta^{\varnothing}{}_{\nu}$, regardless of the specific lattice gas or collision rule.

Equation (72) can now be rewritten in the form

$$N^{\alpha}(t+\Delta t)=\mathcal{P}^{\alpha}{}_{\beta}K^{\beta}{}_{\gamma}N^{\gamma}(t) \ , \tag{76}$$

where K is an operator expressing the complete collision part of the time development, given by

$$K^{\beta}{}_{\gamma}=\prod_{\mathbf{x}\in L_{\beta}} V^{\beta\mathbf{x}}{}_{\gamma_{\mathbf{x}}} \; . \tag{77}$$

We now transform the exact equation of motion (76) into an equation of motion for the CCF's. Using the functions f and g from Eqs. (69) and (70) to convert from means to CCF's and back, Eq. (76) can be rewritten as

$$\Gamma^{\alpha}(t+\Delta t)=g^{\alpha}(\mathcal{P}^{*}{}_{\beta}K^{\beta}{}_{\gamma}f^{\gamma}(\Gamma^{*})) \; .$$

However, note that from the definitions of f and g, a permutation on the bit labels can be performed before or after calculating means from CCF's or vice versa, without changing the result. Thus g and $\mathcal{A}$ commute and this equation can be rewritten as

$$\Gamma^{\alpha}(t+\Delta t)=\mathcal{P}^{\alpha}{}_{\beta}\Phi^{\beta}(\Gamma^{*}) \tag{78}$$

where

$$\Phi^{\beta}(\Gamma^{*})\equiv g^{\beta}(K^{*}{}_{\gamma}f^{\gamma}(\Gamma^{*})) \; .$$

Since we have chosen to expand around a Gibbsian equilibrium, all of the quantities $\Gamma^{\hat{\alpha}}$ are of order ϵ (recall $|\hat{\alpha}|\geq 2$). To perform a complete analysis of the system in the scaling limit, we need only keep terms of first order in ϵ in these quantities and hence in the expression $\Phi^{\hat{\beta}}(\Gamma^{*})$. This is essentially because the conservation equation (13) is linear and is unchanged by the inclusion of correlations; the effect of correlations appears only at order ϵ in Eq. (12). [The ordering of $\Gamma^{\hat{\alpha}}$ at $O(\epsilon)$ will be assumed throughout this paper. Of course, there will be $O(\epsilon^{2})$ contributions as well. These terms are irrelevant in the scaling limit unless there is a divergence in their coefficients. We know of no lattice gases that have such a divergence at $O(\epsilon^{2})$ that do not already diverge at $O(\epsilon)$.] We can linearize Eq. (78) in an analogous fashion to the linearization of the Boltzmann equation in Eq. (71) to get

$$\Gamma^{\hat{\alpha}}(t+\Delta t)=\mathcal{P}^{\hat{\alpha}}{}_{\hat{\beta}}[\epsilon\mathcal{K}^{\hat{\beta}}{}_{a}N_{1}^{a}(t)+\mathcal{K}^{\hat{\beta}}{}_{\hat{\gamma}}\Gamma^{\hat{\gamma}}(t)] \; , \tag{79}$$

where

$$\mathcal{K}^{\beta}{}_{\gamma}=\left.\frac{\partial\Phi^{\beta}}{\partial\Gamma^{\gamma}}\right|_{0}=\left.\frac{\partial g^{\beta}}{\partial N^{\sigma}}\right|_{0}K^{\sigma}{}_{\tau}\left.\frac{\partial f^{\tau}}{\partial\Gamma^{\gamma}}\right|_{0} \; . \tag{80}$$

Similarly, when we include the effects of correlations to order ϵ in Eq. (78) for $\alpha=\{a\}$, the dynamical equation for $N^{a}=\Gamma^{a}$ becomes

$$N^{a}(t+\Delta t)=\mathcal{P}^{a}{}_{b}\{N^{b}(t)+\epsilon[\mathcal{K}^{b}{}_{c}-\delta^{b}{}_{c}]N_{1}^{c}(t)+\mathcal{K}^{b}{}_{\hat{\gamma}}\Gamma^{\hat{\gamma}}(t)\} \; . \tag{81}$$

Note that if we set $\Gamma^{\hat{\alpha}}=0$ in this equation, we get back the linearized Boltzmann equation (71) since

$$\mathcal{K}^{b}{}_{c}-\delta^{b}{}_{c}=\delta^{\mathbf{x}(b)}{}_{\mathbf{x}(c)}J^{i(b)}{}_{i(c)} \; . \tag{82}$$

Inserting Eq. (79) repeatedly into Eq. (81), we can now write an expression for the mean occupation number of a certain bit of the system at position $\mathbf{x}$ and time $t+\Delta t$, written as an infinite sum of terms, each of which is a function of the quantities N_0 and N_1 at nearby lattice sites $\mathbf{x}'$ and at previous time steps t'. As we consider terms in this series with more and more factors of $\mathcal{P}\mathcal{K}$, the positions and times at which these quantities are evaluated will differ from $\mathbf{x}$ and t by greater amounts. However, for any given term in the series, the means $N_{0}^{a(i,\mathbf{x}')}(t')$ and $N_{1}^{a(i,\mathbf{x}')}(t')$ can be replaced by $N_{0}^{a(i,\mathbf{x})}(t)$ and $N_{1}^{a(i,\mathbf{x})}(t)$ and the expression (84) will only change by a quantity of order ϵ, since spatial derivatives are ordered as ϵ and temporal derivatives are ordered as ϵ^{2}. Such a modification for a finite number of terms does not change the behavior of the system in the hydrodynamic limit. In fact, it follows that whenever the sum of terms in Eq. (84) converges on a scale that goes to zero in the hydrodynamic limit, we can drop all the spatial and temporal variations in the single-particle means. The resulting exact equation of motion for the quantities N^{a} is

$$N^{a}(t+\Delta t)=\mathcal{P}^{a}{}_{b}[N^{b}(t)+\epsilon\mathcal{J}^{b}{}_{c}N_{1}^{c}(t)] \; , \tag{83}$$

where

$$\begin{aligned}\mathcal{J}^{b}{}_{c}={}&\delta^{\mathbf{x}(b)}{}_{\mathbf{x}(c)}J^{i(b)}{}_{i(c)}\\&+\mathcal{K}^{b}{}_{\hat{\alpha}}[\mathcal{P}^{\hat{\alpha}}{}_{\hat{\beta}}\mathcal{K}^{\hat{\beta}}{}_{c}+\mathcal{P}^{\hat{\alpha}}{}_{\hat{\beta}}\mathcal{K}^{\hat{\beta}}{}_{\hat{\gamma}}(\mathcal{P}^{\hat{\gamma}}{}_{\hat{\delta}}\mathcal{K}^{\hat{\delta}}{}_{c}+\cdots)]+O(\epsilon) \; ,\end{aligned} \tag{84}$$

where all $\mathcal{K}$'s in $\mathcal{J}$ are evaluated at the point $\mathbf{x}$ and the time t. Similarly, removing the spatial dependence of c, Eq. (83) can be rewritten in precisely the form of Eq. (71), where J is replaced by the renormalized matrix

$$\tilde{J}^{i}{}_{j}(\mathbf{x})=\sum_{\mathbf{y}\in L}\mathcal{J}^{a(i,\mathbf{x})}{}_{a(j,\mathbf{y})}+O(\epsilon) \; . \tag{85}$$

It is important to note that the above argument breaks down when the sum (84) is divergent. It is a well-known result of continuum kinetic theory [18] that velocity autocorrelation functions of fluid systems (conserved mass and momentum) decay with time as $t^{-D/2}$, while those of diffusive systems (conserved mass only) decay as $t^{-1-D/2}$. Since transport coefficients are given by the time integral of the velocity autocorrelation function, it follows that diffusivity converges for all $D\geq 1$, but that viscosity diverges logarithmically for $D=2$. Likewise for lattice gases, when the time series of correlations converges sufficiently rapidly, all zeroth-order means appearing in Eq. (84) can be evaluated at the same point in space and time because the terms that dominate this series involve quantities from a region of space and time that goes to zero in the scaling limit. This is the case for diffusive lattice gases for $D\geq 1$ and for fluid lattice gases for $D\geq 3$. Thus we expect that our 1D3P, 2D4P, and Burgers equation examples will have no convergence problems since they are all diffusive lattice gases in one or two dimensions, and this expectation is borne out by explicit calculations of the diagrammatic sums.

The FHP model, on the other hand, is a two-dimensional fluid and so its time series of correlations diverges logarithmically with the size of the system. The form of this logarithmic divergence can also be derived directly from the diagrammatic sums. One might expect this divergence to mean that the sum (84) is nonlocal and gives rise to an integral equation in the continuum limit, but there is a simplification for incompressible fluids (or for any system for which the conserved quantities are ordered as in Sec. III H) because the zeroth-order equilibrium is spatially invariant. In this case, the zeroth-order means can simply be replaced by their universal values in spite of the logarithmic divergence. For a compressible fluid, on the other hand, the effects of large scale variations in the $N^{a(i,\mathbf{x})}$'s must be considered and the full equation of motion might well be integro-differential in character. In general, for lattice gases where the sum (84) is divergent, one must be quite careful about the analysis.

Now that we have rewritten the exact dynamical equation in a form commensurate with the original form of the lattice Boltzmann equation, the renormalized transport coefficients for the theory can be related to the eigenvalues of the matrix $\tilde{J}^i{}_j$ in the same way that the original (Boltzmann) transport coefficients were related to the eigenvalues of the matrix $J^i{}_j$. Thus, if we can compute the matrix $\tilde{J}^i{}_j$ exactly, we can also compute the exact renormalized transport coefficients. Most of the rest of this paper is devoted to methods of calculating and approximating the matrix $\tilde{J}^i{}_j$ and applications to specific lattice gases.

D. Factorization of the collision operator

In the next two subsections we shall show that expression (84) for $\mathcal{J}$ can be written in a diagrammatic notation, allowing us to perform a perturbative calculation of $\mathcal{J}$ by summing over "Feynman diagram"-like objects, where the contribution from each diagram is just the product of factors associated with its vertices. The principal observation that allows this reduction is that the collision operator $\mathcal{K}^\alpha{}_\beta$ is factorizable. We devote this subsection to demonstrating the exact form of this factorization.

Theorem 2. For fixed α and β, $\mathcal{K}^\alpha{}_\beta$ can be broken down into a product of contributions from distinct vertices. Explicitly,

$$\mathcal{K}^\alpha{}_\beta = \prod_{\mathbf{x}\in L_\alpha} \mathcal{V}^{\alpha_\mathbf{x}}{}_{\beta_\mathbf{x}} , \tag{86}$$

where the correlation vertex coefficients (CVC's) $\mathcal{V}$ are defined by

$$\mathcal{V}^{\alpha_\mathbf{x}}{}_{\beta_\mathbf{x}} = \sum_{\mu,\nu} (-1)^{|\alpha_\mathbf{x}\setminus\mu|} \left[\prod_{i\in(a_\mathbf{x}\setminus\mu)} N_0^i \right] \times \left[\prod_{j\in(\nu\setminus\beta_\mathbf{x})} N_0^j \right] V^\mu{}_\nu , \tag{87}$$

with the sum taken over $\mu\subseteq\alpha_\mathbf{x}$ and $\nu\supseteq\beta_\mathbf{x}$, $\nu\subseteq B$.

Proof. To prove the theorem, we need only compute the derivatives of the means and CCF's with respect to one another, evaluated at the equilibrium point. From the definitions (69) and (70), it is clear that when $\beta\not\subseteq\alpha$, $\partial g^\alpha/\partial N^\beta = \partial f^\alpha/\partial\Gamma^\beta = 0$. When $\beta\subseteq\alpha$, it is also fairly straightforward to compute from Eq. (69)

$$\left.\frac{\partial f^\alpha}{\partial\Gamma^\beta}\right|_0 = \prod_{a\in(\alpha\setminus\beta)} N_0^{i(a)} = \prod_{\mathbf{x}\in L_\alpha} \prod_{i\in(\alpha_\mathbf{x}\setminus\beta_\mathbf{x})} N_0^i . \tag{88}$$

Similarly, when $\beta\subseteq\alpha$, the derivatives $\partial g^\alpha/\partial N^\beta$ are given by

$$\left.\frac{\partial g^\alpha}{\partial N^\beta}\right|_0 = \prod_{a\in\alpha\setminus\beta} (-N_0^{i(a)}) = \prod_{\mathbf{x}\in L_\alpha} \prod_{i\in\alpha_\mathbf{x}\setminus\beta_\mathbf{x}} (-N_0^i) . \tag{89}$$

Substituting Eqs. (77), (88), and (89) into Eq. (80), we get

$$\mathcal{K}^\alpha{}_{\cdot\beta} = \sum_{\gamma\subseteq\alpha,\zeta\supseteq\beta} \left[\prod_{\mathbf{x}\in L_\alpha} \prod_{i\in(\alpha_\mathbf{x}\setminus\gamma_\mathbf{x})} (-N_0^i) \right] \left[\prod_{\mathbf{x}\in L_\gamma} V^{\gamma_\mathbf{x}}{}_{\zeta_\mathbf{x}} \right] \times \left[\prod_{\mathbf{x}\in L_\zeta} \prod_{j\in(\zeta_\mathbf{x}\setminus\beta_\mathbf{x})} N_0^j \right] .$$

Since $\gamma\subseteq\alpha$, clearly $L_\gamma\subseteq L_\alpha$. The fact that $V^\varnothing{}_\nu=0$ when $\nu\neq 0$ implies that all terms with $L_\zeta\not\subseteq L_\gamma$ vanish, so we can restrict the sum over ζ to only those ζ with $L_\zeta\subseteq L_\alpha$. In this case for $\mathbf{x}\notin L_\gamma$, clearly $V^{\gamma_\mathbf{x}}{}_{\zeta_\mathbf{x}} = V^\varnothing{}_\varnothing = 1$ or $V^{\gamma_\mathbf{x}}{}_{\zeta_\mathbf{x}}=0$, and for $\mathbf{x}\notin L_\zeta$, clearly $\zeta_\mathbf{x}\setminus\beta_\mathbf{x}=\varnothing$, so we can replace all the products with products over $\mathbf{x}\in L_\alpha$, giving

$$\mathcal{K}^\alpha{}_\beta = \sum_{\gamma,\zeta} \prod_{\mathbf{x}\in L_\alpha} \prod_{i\in(\alpha_\mathbf{x}\setminus\gamma_\mathbf{x})} (-N_0^i) V^{\gamma_\mathbf{x}}{}_{\zeta_\mathbf{x}} \prod_{i\in(\zeta_\mathbf{x}\setminus\beta_\mathbf{x})} N_0^i , \tag{90}$$

where the sum is over all $\gamma\subseteq\alpha$ and all ζ satisfying $L_\zeta\subseteq L_\alpha$ and $\zeta\supseteq\beta$. For each $\mathbf{x}$, however, this means that $\gamma_\mathbf{x}$ and $\zeta_\mathbf{x}$ are summed over all $\gamma_\mathbf{x}\subseteq\alpha_\mathbf{x}$ and $\zeta_\mathbf{x}\supseteq\beta_\mathbf{x}$. Since the $\gamma_\mathbf{x}$ and $\zeta_\mathbf{x}$ are independent for different $\mathbf{x}$, a distributive rule can be applied to Eq. (90), giving $\mathcal{K}^\alpha{}_\beta$ in exactly the form stated in Theorem 2, so the proof is complete. ■

E. Diagrammatics

Using the result from the preceding subsection, it is possible to express every term in $\mathcal{J}$ in diagrammatic form. A generic term in $\mathcal{J}^a{}_b$ is of the form

$$\mathcal{K}^{\alpha^k}{}_{\beta^k}\mathcal{P}^{\beta^k}{}_{\alpha^{k-1}}\mathcal{K}^{\alpha^{k-1}}{}_{\beta^{k-1}} \cdots \mathcal{P}^{\beta^2}{}_{\alpha^1}\mathcal{K}^{\alpha^1}{}_{\beta^1} \tag{91}$$

with α^i and β^i fixed (i.e., not summed over) and $|\alpha^i|,|\beta^i|\geq 2$, except for the end points where $\alpha^k=\{a\}$ and $\beta^1=\{b\}$.

We define a *diagram* T by an integer $k(T)$, which we refer to as the *length* of the diagram T, and a function $\alpha_T(\tau)$, where for each $\tau\in\{0,\ldots,k\}$, $\alpha_T(\tau)\subseteq\mathcal{B}$. Geometrically, we associate each $a\in\alpha_T(\tau)$ with a *virtual particle* (VP) moving from $(\mathbf{x}(a),\tau)$ to $(\mathbf{x}(a)+\mathbf{c}^{i(a)},\tau+1)$ on the lattice $\Lambda_{k+1}=L\times\{0,\ldots,k+1\}$. We refer to $\alpha_T(\tau)$ as the set of *outgoing* VP's for the diagram T.

It is natural to define a corresponding set of *incoming* VP's for $\tau>0$ by $\beta_T(\tau)=\{b\colon a(i(b),\mathbf{x}(b)-\mathbf{c}^{i(b)})\in\alpha_T(\tau-1)\}$. We also define $\sigma_T(\tau)=|\alpha_T(\tau)|$ to be the total number of outgoing VP's for each value of τ. Finally, given a diagram T, we can define a weight function

$$W(T)=\prod_{\mathbf{x}\in L}\prod_{1\le\tau\le k(T)}\mathcal{V}^{\alpha_T(\tau)_{\mathbf{x}}}{}_{\beta_T(\tau)_{\mathbf{x}}}$$

by taking the product of $\mathcal{V}$ over all vertices.

The term (91) can now be represented by the diagram T with $\alpha_T(\tau)=\alpha^\tau$, where for consistency α^0 is defined to be the unique set with $\mathcal{P}^{\beta^1}{}_{\alpha^0}=1$. When $\tau\neq 0$, $\mathcal{P}^{\beta^{\tau+1}}{}_{\alpha^\tau}=1$, so $\beta_T(\tau)=\beta^\tau$ for all τ. It follows that the contribution from the term (91) is exactly given by $W(T)$. Thus we can rewrite expression (84) for $\mathcal{J}^a{}_b$ as a sum over diagrams

$$\mathcal{J}^a{}_b=\sum_{k=1}^{\infty}\sum_{T\in\mathcal{T}^a{}_b(k)}W(T)\ , \tag{92}$$

where in general we define the set of diagrams $\mathcal{T}^\alpha{}_\beta(k)$ by

$$\mathcal{T}^\alpha{}_\beta(k)=\{T\colon k=k(T),\ \sigma_T(l)>1 \text{ for } 1\le l<k,\ \alpha_T(k)=\alpha,\ \beta_T(1)=\beta\}\ .$$

Note that $\mathcal{V}^{\varnothing}{}_\nu=\delta^{\varnothing}{}_\nu$, so any diagram with incoming VP's at $(\mathbf{x},t)$ but no outgoing VP's has weight zero. For many lattice gases certain other vertex factors $\mathcal{V}^\mu{}_\nu$ also vanish; diagrams with such vertices can be dropped from the sum (92). From Eq. (85), $\tilde{J}$ can now be written as a sum over diagrams in the same fashion as $\mathcal{J}$,

$$\tilde{J}^i{}_j(\mathbf{x})=\sum_{k=1}^{\infty}\sum_{T\in\mathcal{T}^i{}_j(\mathbf{x},k)}W(T)\ , \tag{93}$$

where the set of diagrams to be summed over is given by

$$\mathcal{T}^i{}_j(\mathbf{x},k)=\bigcup_{b\colon i(b)=j}\mathcal{T}^{a(i,\mathbf{x})}{}_b(k)\ .$$

We shall find it useful later to generalize this set of diagrams to the sets of diagrams

$$\mathcal{T}^\mu{}_\nu(\mathbf{x},k)=\{T\colon k=k(T),\ \sigma_T(l)>1 \text{ for } 1\le l<k,\ |L_{\alpha_T(0)}|=1,\ L_{\alpha_T(k)}=\{\mathbf{x}\},\ \mu(\alpha_T(k))=\mu,\ \mu(\alpha_T(0))=\nu\}\ ,$$

where we have used the notation

$$\mu(\{a_1,\dots,a_j\})=\{i(a_1),\dots,i(a_j)\}\ .$$

Example. As a simple example of the diagrammatic notation, consider the allowed diagrams for the 1D3P lattice gas considered in Sec. IV A. The complete set of diagrams needed to compute the $k=3$ correction to $\tilde{J}^0{}_0$ is the set of diagrams T_1-T_4 represented in Fig. 4, along with the diagrams achieved by reflecting T_1 and T_2 across the x axis. The weight of diagram T_2, for example, is $W(T_2)=\mathcal{V}^0{}_{\hat{-}}\mathcal{V}^+{}_-\mathcal{V}^0{}_0\mathcal{V}^{\hat{+}}{}_0$. Note that this diagram corresponds precisely to the term computed in the example of Sec. V. The coefficients $-p, pf, 1-2pf, -pf+pf^2$ computed in that calculation are precisely the CVC's in $W(T_2)$. We shall compute the remaining vertex factors $\mathcal{V}^\mu{}_\nu$ for this lattice gas in Sec. VII A and we shall see that the contribution from diagram T_3 in fact vanishes.

F. Approximations

We have so far managed to write the exact formula for the hydrodynamic equations in the scaling limit only in terms of an infinite formal series. The natural next question to confront is whether this series can be summed. We would like to know whether the series is finite, and if we cannot sum the full series, at least we would like to find a set of reasonable approximations that we can make to truncate the series to one that is summable. The questions of convergence are rather difficult and we shall not address them here in full generality; in general, the convergence properties of the series depend on the form of the conserved quantities in the system. A variety of methods for performing partial sums of infinite series of diagrams while retaining physically important terms has been applied to related problems in quantum field theory and quantum many-body theory [34,35]. We shall describe here several particular approximation methods that are useful for the kind of series that arises for known lattice gases.

1. Short-τ and small-l truncations

The simplest useful approximations involve truncating the sum (92) to a finite number of terms by putting an upper bound on either the number of time steps or the number of distinct nontrivial vertices allowed in each diagram. In the first case, the expression for the renormalized J matrix is

$$\tilde{J}^{(\tau)i}{}_j(\mathbf{x})=\sum_{k=1}^{\tau}\sum_{T\in\mathcal{T}^i{}_j(\mathbf{x},k)}W(T)\ ,$$

where the diagrams summed over are the same as those summed in Eq. (93). Since for each fixed value of k there is a finite number of allowed diagrams, this sum is finite. We refer to this approximation as the *short-τ approximation.*

It is important to distinguish the short-τ approximation from the transient effects encountered when a lattice gas is first started from random initial conditions. In the short-τ approximation, we still assume that the lattice gas has run for a sufficiently long time that the higher corre-

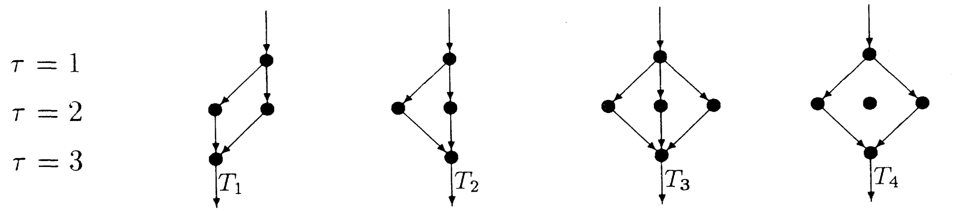


FIG. 4. $k=3$ diagrams for a 1D lattice gas with three bits per site.

lations have had a chance to develop from the random initial conditions in which they are artificially suppressed. The point of the short-τ approximation is to additionally assume that, in this asymptotic state, the dominant contributions come from diagrams with short temporal extension. This is very different from the goal of describing the transient startup of the lattice gas. In fact, the formalism used here can easily be extended to describe the dynamics of correlations in the transient period [36]. In this paper, however, we concentrate on asymptotic properties of lattice-gas dynamics, such as the transport coefficients, and, for certain lattice-gas models, the short-τ approximation is useful to this end.

In the second case, we allow k to be arbitrary, but allow only diagrams where the total number of vertices $(\mathbf{x},k')$ with nonempty outgoing sets $\alpha_T(k')_{\mathbf{x}}$ is less than or equal to some fixed number l. We denote the sum restricted to these diagrams by $\tilde{J}^{[l]i}{}_j$. Again, there is only a finite number of such diagrams in this sum, which means that this sum must also be finite. This approximation is analogous to the weak-coupling expansions in quantum field theory, although in this case the coupling constants $\mathcal{V}^{\mu}{}_{\nu}$ are usually not particularly small. The short-τ and small-l truncations give good consecutive approximations for many lattice gases. In either of these two approximations, the Boltzmann approximation can be recovered, by taking $\tau=1$ or $l=1$.

2. BBGKY truncations

Another good class of approximations, in which a reduced but still infinite set of diagrams is summed, corresponds to truncations of the BBGKY hierarchy of equations. Such an approximation involves neglecting q-CCF's with $q>n$ for some fixed value of n. In our diagrammatic formalism, this amounts to restricting the sum to diagrams with $\sigma_T(k')\le n$ for $1\le k'\le k$. For example, with $n=2$, diagram T_3 of Fig. 4 would be neglected. Whereas the computational complexity of including all diagrams in the complete sum grows exponentially in k, that of the truncated BBGKY approximations grows polynomially, so the latter are computationally more tractable.

3. Ring approximation

The $n=2$ version of the BBGKY approximation is closely related to the *ring approximation.* The ring approximation is made by neglecting interactions between two propagating correlated quantities except at the initial and final vertices of a diagram. It is generally possible to calculate a closed-form expression for the infinite sum of diagrams corresponding to this approximation. Furthermore, it is usually fairly easy to calculate the asymptotic form of this approximation as $k\to\infty$. This calculation often captures the most significant part of the long-term renormalization effects. In particular, for certain lattice gases that model two-dimensional fluid systems, the ring approximation diverges logarithmically in $|L|$, which is in agreement with predictions from other theoretical frameworks [23] and also with observed behavior [37].

In Sec. VIII we shall apply the different approximation methods described here to the 1D3P lattice gas and compare the results from these approximations with computer experimental results.

G. Eigenvalue renormalization

Within the framework of the formalism developed in the previous subsections, we can now demonstrate that for a large class of lattice gas models, the effects of correlations are to renormalize only the eigenvalues of the J matrix and not to change the eigenvectors. This result follows from a pair of fairly simple theorems.

Theorem 3. The finite matrix $C^{(\tau)i}{}_j=\tilde{J}^{(\tau)i}{}_j-J^i{}_j$ of corrections to the J matrix can be restricted to be a matrix in the space of kinetic eigenvectors of J, i.e., if $\nu\in H$, then

$$q_i^{\nu}(\tilde{J}^{(\tau)i}{}_j-J^i{}_j)=(\tilde{J}^{(\tau)i}{}_j-J^i{}_j)q^j_{\nu}=0\ .$$

Proof. From Eqs. (84) and (86), it will clearly suffice to show that $q_i^{\nu}\mathcal{V}^i{}_{\hat{\mu}}=\mathcal{V}^{\hat{\mu}}{}_j q^j_{\nu}=0$ for every $\hat{\mu}\subseteq B$ with $|\hat{\mu}|\ge 2$.

We first demonstrate this sufficient condition for the right hydrodynamic eigenvectors q^i_{ν}. We showed in Sec. III E that q^i_{ν} was a right eigenvector of the J matrix with eigenvalue 0 by differentiating the identity $\Omega^i(N_0^*)=0$, which holds for any equilibrium, with respect to the parameters α_{ν} of the equilibrium. We can similarly show that q^i_{ν} is a null right eigenvector of $\mathcal{V}^{\hat{\mu}}{}_i$ by using the stability of the Boltzmann equilibria. The stability of the local Boltzmann equilibrium tells us that at each lattice site,

$$g^{\hat{\mu}}\left[\sum_{\rho\subseteq B}V^*{}_{\rho}\prod_{i\in\rho}N_0^i\right]=0\ .$$

Differentiating this equation with respect to the parameter α_{ν} of the local Boltzmann equilibrium gives

$$0=\sum_{\xi\subseteq\hat\mu,\rho\subseteq B}\left[\prod_{j\in\hat\mu\setminus\xi}-N_0^j\right]V^{\xi}{}_{\rho}\left[\sum_{i\in\rho}\left[\prod_{k\in\rho\setminus i}N_0^k\right]q^i_{\nu}\right]$$
$$=\mathcal{V}^{\hat\mu}{}_{i}q^i_{\nu}\ ,$$

as desired.

Next, consider the left hydrodynamic eigenvector q_i^{ν}. From Eq. (87), we have

$$\mathcal{V}^{i}{}_{\hat\mu}=\sum_{\nu\supseteq\hat\mu}\left[\prod_{j\in\nu\setminus\hat\mu}N_0^j\right]V^{i}{}_{\nu}\ .$$

Since $q_i^{\nu}N^i$ is a conserved quantity for any value of N^i, we have

$$q_i^{\nu}\sum_{\mu\subseteq B}V^{i}{}_{\mu}\left[\prod_{j\in\mu}N_0^j\right]=q_i^{\nu}N_0^i$$

for arbitrary N_0^i, so $q_i^{\nu}V^{i}{}_{\hat\mu}=q_i^{\nu}\mathcal{V}^{i}{}_{\hat\mu}=0$ for all $\hat\mu\subseteq B$ with $|\hat\mu|\geq 2$. ■

Theorem 4. If there exists a symmetry Σ of a lattice gas that can be expressed as a combination of a permutation $\dot\Sigma^{\mathbf{x}}{}_{\mathbf{y}}$ on the lattice L fixing a point $\mathbf{x}$ and an independent permutation $\bar\Sigma^{i}{}_{j}$ on the bit set B, where the zeroth-order Boltzmann equilibrium at $\mathbf{x}$ satisfies $\bar\Sigma^{i}{}_{j}N_0^j(\mathbf{x})=N_0^i(\mathbf{x})$, then $\bar\Sigma$ commutes with J and $\tilde J^{(\tau)}$, i.e.,

$$\bar\Sigma^{i}{}_{j}J^{j}{}_{k}(\mathbf{x})-J^{i}{}_{j}(\mathbf{x})\bar\Sigma^{j}{}_{k}=\bar\Sigma^{i}{}_{j}\tilde J^{(\tau)j}{}_{k}(\mathbf{x})-\tilde J^{(\tau)i}{}_{j}(\mathbf{x})\bar\Sigma^{j}{}_{k}=0\ .$$

Proof. The condition that Σ is a symmetry of the lattice gas with the given product structure asserts that $\Sigma^{a}{}_{b}=\bar\Sigma^{i(a)}{}_{i(b)}\dot\Sigma^{\mathbf{x}(a)}{}_{\mathbf{x}(b)}$ is a permutation matrix on all the bits of the system, which can be extended to a permutation matrix $\Sigma^{\alpha}{}_{\beta}$ on subsets of B, satisfying

$$(\Sigma^{-1})^{\alpha}{}_{\beta}\mathcal{P}^{\beta}{}_{\gamma}\Sigma^{\gamma}{}_{\delta}=\mathcal{P}^{\alpha}{}_{\delta}$$

and

$$(\Sigma^{-1})^{\alpha}{}_{\beta}K^{\beta}{}_{\gamma}\Sigma^{\gamma}{}_{\delta}=K^{\alpha}{}_{\delta}\ .$$

Since by their definitions the functions f and g connecting means and CCF's are invariant under permutations, it follows from Eq. (80) and the invariance of the local Boltzmann equilibrium at $\mathbf{x}$ that

$$(\Sigma^{-1})^{\alpha}{}_{\beta}\mathcal{K}^{\beta}{}_{\gamma}\Sigma^{\gamma}{}_{\delta}=\mathcal{K}^{\alpha}{}_{\delta}\ ,$$

where we assume that all zeroth-order single-particle means are evaluated at $\mathbf{x}$, as in the diagrammatic expansion. It then follows from Eqs. (82), (84), and the fact that $\delta^{\alpha}{}_{\beta}$ commutes with Σ that

$$(\Sigma^{-1})^{a}{}_{b}\mathcal{J}^{b}{}_{c}\Sigma^{c}{}_{d}=\mathcal{J}^{a}{}_{d}$$

and

$$(\bar\Sigma^{-1})^{i}{}_{j}J^{j}{}_{k}(\mathbf{x})\bar\Sigma^{k}{}_{l}=J^{i}{}_{l}(\mathbf{x})\ ,$$

proving the first part of the theorem. From the constraint that $\dot\Sigma$ leave the point $\mathbf{x}$ fixed, we have

$$\tilde J^{i}{}_{l}(\mathbf{x})=\sum_{\mathbf{w}}\mathcal{J}^{a(i,\mathbf{x})}{}_{a(l,\mathbf{w})}$$
$$=\sum_{\mathbf{w}}(\dot\Sigma^{-1})^{\mathbf{x}}{}_{\mathbf{y}}(\bar\Sigma^{-1})^{i}{}_{j}\mathcal{J}^{a(j,\mathbf{y})}{}_{a(k,\mathbf{z})}\bar\Sigma^{k}{}_{l}\dot\Sigma^{\mathbf{z}}{}_{\mathbf{w}}$$
$$=\sum_{\mathbf{z}}(\bar\Sigma^{-1})^{i}{}_{j}\mathcal{J}^{a(j,\mathbf{x})}{}_{a(k,\mathbf{z})}\bar\Sigma^{k}{}_{l}$$
$$=(\bar\Sigma^{-1})^{i}{}_{j}\tilde J^{j}{}_{k}(\mathbf{x})\bar\Sigma^{k}{}_{l}\ ,$$

so the second assertion of the theorem is proven. ■

Corollary 1. If the kinetic eigenvalues of $\tilde J^{(\tau)}$ converge as $\tau\to\infty$, then the sequence $\{\tilde J^{(\tau)i}{}_{j}\}$ converges as $\tau\to\infty$ and Theorems 3 and 4 hold in this limit, that is,

$$q_i^{\nu}(\tilde J^{i}{}_{j}-J^{i}{}_{j})=(\tilde J^{i}{}_{j}-J^{i}{}_{j})q^j_{\nu}=0\quad\text{for }\nu\in H$$

and

$$\bar\Sigma^{i}{}_{j}J^{j}{}_{k}-J^{i}{}_{j}\bar\Sigma^{j}{}_{k}=\bar\Sigma^{i}{}_{j}\tilde J^{j}{}_{k}-\tilde J^{i}{}_{j}\bar\Sigma^{j}{}_{k}=0$$

for $\bar\Sigma^{i}{}_{j}$, as in Theorem 4.

Note that if the sequence $\{\tilde J^{(\tau)}\}$ does not converge, then neither do the kinetic eigenvalues, and the theory breaks down in the continuum limit.

For a wide class of lattice gases, including all the lattice gases described in Sec. IV A, these two theorems suffice to demonstrate that the eigenvectors of the $\tilde J$ matrix coincide with those of J, so that the only effect of correlations is to renormalize the eigenvalues of J. The essential point is that we can classify the eigenvectors of J by their transformation properties under the group of symmetries of the lattice gas. Theorem 4 asserts that $\tilde J$ can only mix eigenvectors with identical symmetry properties. Thus, if no two kinetic eigenvectors of J share the same symmetry properties, then $\tilde J$ must be diagonal with respect to the basis of eigenvectors of J. More generally, if the representation of the group of symmetries on the space of kinetic eigenvectors of J breaks up into irreducible representations in such a way that no irreducible representation appears more than once, then $\tilde J$ is diagonal with respect to the eigenvectors of J.

As a simple example, consider the 1D3P diffusive lattice gas. The right kinetic eigenvectors of J are

$$q_2=\tfrac{1}{2}\begin{bmatrix}-1\\0\\+1\end{bmatrix},\quad q_3=\tfrac{1}{6}\begin{bmatrix}-1\\+2\\-1\end{bmatrix}\ .$$

Under the symmetry transformation $\mathbf{x}\to-\mathbf{x}$, $+\leftrightarrow-$, these eigenvectors transform with eigenvalues $\Sigma^{2}{}_{2}=-1$ and $\Sigma^{3}{}_{3}=+1$. Thus these eigenvectors cannot be mixed by $\tilde J$ and so their eigenvalues are separately renormalized. Explicitly, in matrix notation, with respect to the basis q_i, we have

$$\tilde J=\begin{bmatrix}0&0&0\\0&j^{2}{}_{2}&j^{2}{}_{3}\\0&j^{3}{}_{2}&j^{3}{}_{3}\end{bmatrix},\quad\bar\Sigma=\begin{bmatrix}+1&0&0\\0&-1&0\\0&0&+1\end{bmatrix}\ .$$

By Theorem 4, $\tilde J$ commutes with $\bar\Sigma$, so $j^{2}{}_{3}=j^{3}{}_{2}=0$.

For most standard lattice gases, a similar analysis of the symmetry properties of the eigenvectors of J shows that no irreducible representation of the symmetry group appears more than once, so that the eigenvalues of J are renormalized in a straightforward fashion. For those lattice gases where this cannot be shown, it is necessary to repeat the entire Chapman-Enskog analysis using the renormalized $\tilde{J}$ matrix. Note that Theorem 4 implies that any eigenvectors of J that lie in the same irreducible representation of the symmetry group must have identical eigenvalues in the matrices J and also in $\tilde{J}$.

H. Renormalization effects and higher-order collision operators

We conclude this section with a discussion of the effects of the higher-order collision operators $\epsilon\omega_1^i$ and $\epsilon^2\omega_2^i$ in the full kinetic theory. We show that the second-order term only appears in the source term for the hydrodynamic equation as in Eq. (40) and does not generate exact renormalization effects. On the other hand, we find that the first-order collision operator not only appears in the advection coefficient as in Eq. (38), but generates a set of additional correlations that modify the advection coefficient by effectively renormalizing the components of the first-order collision operator itself.

We begin by discussing the second-order term $\epsilon^2\omega_2^i$. This part of the collision operator appears only in the first-order conservation equation (37). The corrections to this term due to correlations are of one higher order in ϵ and can clearly be neglected in the entire analysis. Thus inclusion of this term only generates the source term in Eq. (37) in the manner described in Sec. III G.

Now we consider the effects of including a first-order term $\epsilon\omega_1^i$ in the collision operator. Recall that this term is restricted to obey the conservation laws, but is not required to satisfy semidetailed balance. Because this part of the collision operator obeys the conservation laws it does not appear directly in the first-order conservation equation. It does appear in the linearized Boltzmann equation (29), but its corrections due to correlations are again of higher order in ϵ.

At this point, one might imagine that inclusion of the first-order term in the collision operator does not necessitate any further modification to the exact hydrodynamic equation in the scaling limit other than the effects described in Sec. III. However, this is not the case. In fact, the inclusion of this term in the collision operator has a nontrivial effect on Eq. (79), which describes the propagation of correlated quantities in the system.

Equation (79) gives an expression to order ϵ for $\Gamma^{\hat{\alpha}}$ at time $t+\Delta t$ in terms of quantities at time t. In the derivation of Eq. (79), we used the fact that the zeroth-order means N_0^i describe a local Boltzmann equilibrium that does not generate correlations through the collision operator ω_0^i. When we include the first-order collision operator ω_1^i, we must include the fact that $\epsilon\omega_1^i(N_0^*)$ need not vanish. Thus the correct form of Eq. (79) in this case is

$$\Gamma^{\hat{\alpha}}(t+\Delta t)=\mathcal{P}^{\hat{\alpha}}{}_{\hat{\beta}}[\epsilon\mathcal{K}^{\hat{\beta}}{}_a N_1^a(t)+\mathcal{K}^{\hat{\beta}}{}_{\hat{\gamma}}\Gamma^{\hat{\gamma}}(t)+\epsilon I^{\hat{\beta}}]\ , \quad (94)$$

where we have defined $I^{\hat{\beta}}=0$ whenever $|L_{\hat{\beta}}|>1$ and

$$I^{\hat{\beta}}=I^{\mu}\equiv\sum_{\nu\subseteq\mu}\left[\prod_{i\in\mu\setminus\nu}-N_0^i\right]\sum_{\xi}\left[\frac{\partial}{\partial\epsilon}\bigg|_{\epsilon=0}V^{\nu}{}_{\xi}\right]\prod_{j\in\xi}N_0^j \quad (95)$$

whenever $L_{\hat{\beta}}=\{\mathbf{y}\}$ and $\hat{\beta}_{\mathbf{y}}=\mu(\hat{\beta})=\mu$ for some $\mathbf{y}\in L$; all means N_0 in this equation are evaluated at the point $\mathbf{y}$. In Eq. (95) we have used the collision operator on means $V^{\nu}{}_{\gamma}$ defined by using the collision operator $\omega^i=\omega_0^i+\epsilon\omega_1^i$. However, the CVC's used in Eq. (94) should still be evaluated with respect to the zeroth-order collision operator ω_0^i.

Combining Eqs. (94) and (81) and including the first-order collision operator as in Eq. (29), we get

$$N^a(t+\Delta t)=\mathcal{P}^a{}_b[N^b(t)+\epsilon\mathscr{J}^b{}_c N_1^c(t)+\epsilon\mathcal{J}^b]\ ,$$

where

$$\mathcal{J}^b=\Omega_1^{i(b)}(N_0^*(\mathbf{x}(b)))$$
$$+\mathcal{K}^b{}_{\hat{\alpha}}[\mathcal{P}^{\hat{\alpha}}{}_{\hat{\beta}}I^{\hat{\beta}}+\mathcal{P}^{\hat{\alpha}}{}_{\hat{\beta}}\mathcal{K}^{\hat{\beta}}{}_{\hat{\gamma}}(\mathcal{P}^{\hat{\gamma}}{}_{\hat{\delta}}I^{\hat{\delta}}+\cdots)]\ .$$

By applying the same analysis used in Sec. III, we find that the renormalized hydrodynamic equations for the theory are of the same form as Eq. (37); however, the inclusion of the first-order collision term changes the result for the renormalized advection coefficient to be

$$\mathcal{A}^{\mu}(Q^*)=\frac{c}{\Delta t}\sum_{\nu\in K}\frac{\tilde{\delta}(1)^{\mu}{}_{\nu}\tilde{\mathcal{C}}_1^{\nu}(Q^*)}{(-\tilde{\lambda}^{\nu})}\ ,$$

where the renormalized generalized Kronecker δ function and eigenvalues are defined with respect to the renormalized J matrix and the renormalized collision operator $\tilde{\mathcal{C}}_1^{\nu}$ is given by

$$\tilde{\mathcal{C}}_1^{\nu}(\mathbf{x})=q_i^{\nu}\mathcal{J}^{a(i,\mathbf{x})}\ .$$

Just as for the renormalized J matrix, we evaluate all means N_0 appearing in CVC's and I^{μ} at the point $\mathbf{x}$. This simplification depends again upon the convergence of the infinite series of terms in $\tilde{\mathcal{C}}_1^{\nu}$.

We can express the renormalized collision operator in terms of an infinite diagrammatic sum, analogous to the sum (93) for the renormalized matrix $\tilde{J}$. Specifically, we have

$$\mathcal{J}^a=\Omega_1^{i(a)}+\sum_{k=1}^{\infty}\sum_{T\in\mathcal{T}^{i(a)}{}_{\mu}(\mathbf{x}(a),k)}W(T)I^{\mu}\ .$$

VII. EXAMPLES OF VERTICES AND RENORMALIZATION

We shall now apply the methods of the preceding section to compute the vertex factors for the example lattice gases described in Sec. IV. We also derive expressions for the renormalized transport coefficients for all these lattice gases.

A. 1D3P lattice gas

1. Vertices

Beginning with either the collision operator Eq. (47) or the state transition table (see Sec. IV A) for the 1D3P lattice gas, we can calculate the mean vertex coefficients $V^{\mu}{}_{\nu}$ using Eqs. (73) and (75). The nonzero mean vertex coefficients are given by

$$V^{B}{}_{B} = V^{\varnothing}{}_{\varnothing} = 1, \quad V^{i}{}_{\hat{\jmath}} = p(3\delta^{i}{}_{j} - 1) ,$$
$$V^{i}{}_{j} = \delta^{i}{}_{j}, \quad V^{\hat{\imath}}{}_{\hat{\jmath}} = p + \delta^{i}{}_{j}(1-3p) .$$

Note that since the ensemble-averaged collision operator is invariant under permutations (relabeling) on the bits, the mean vertex coefficients also have this symmetry.

Using the equilibrium value f for the mean occupation numbers N^{i}_{0} [see Eq. (48)], the expression for the CVC's, Eq. (87), reads

$$\mathcal{V}^{\alpha}{}_{\beta} = \sum_{\mu\subseteq\alpha,\nu\supseteq\beta} (-1)^{|\alpha|-|\mu|} f^{|\alpha|+|\nu|-|\mu|-|\beta|} V^{\mu}{}_{\nu} .$$

For instance, we have

$$\mathcal{V}^{\hat{+}}{}_{0} = f(V^{\hat{+}}{}_{\hat{+}} + V^{\hat{+}}{}_{\hat{-}} - V^{0}{}_{0} - V^{-}{}_{0})$$
$$- f^{2}(V^{0}{}_{\hat{+}} + V^{-}{}_{\hat{+}} + V^{0}{}_{\hat{-}} + V^{-}{}_{\hat{-}}) = -pf(1-f) .$$

The remaining nonzero CVC's are given by the equations

$$\mathcal{V}^{B}{}_{B} = \mathcal{V}^{\varnothing}{}_{\varnothing} = 1, \quad \mathcal{V}^{\hat{\imath}}{}_{j} = \delta^{i}{}_{j}3pf(1-f) - pf(1-f) ,$$
$$\mathcal{V}^{i}{}_{j} = pf + \delta^{i}{}_{j}(1-3pf) , \qquad (96)$$
$$\mathcal{V}^{\hat{\imath}}{}_{\hat{\jmath}} = p(1-f) + \delta^{i}{}_{j}(1-3p(1-f)), \quad \mathcal{V}^{i}{}_{\hat{\jmath}} = \delta^{i}{}_{j}3p - p .$$

Note that the CVC's are also symmetric under an arbitrary permutation on the particle labels. The nonvanishing correlation vertex factors are depicted graphically in Fig. 5; only a single vertex is shown in each equivalence class under the permutation symmetry.

2. *Renormalization of diffusivity*

As shown in Sec. VI G, the symmetry of the 1D3P lattice gas under spatial inversion is sufficient to ensure that the effect of correlations is simply to renormalize the kinetic eigenvalues. From the Chapman-Enskog analysis, we know that the diffusivity is given in the hydrodynamic limit by

$$\tilde{D} = \frac{c^2}{3\Delta t}\left[\frac{2}{-\tilde{\lambda}} - 1\right] , \qquad (97)$$

where $\tilde{\lambda}$ is the eigenvalue of the vector $(-1,0,+1)$ in the matrix $\tilde{J}$. In this subsection we shall find the set of diagrams that contribute to the renormalization of λ.

Factoring out the initial and closure vertices, we can write the renormalized matrix $\tilde{J}$ as

$$\tilde{J}^{i}{}_{j}(\mathbf{x}) = J^{i}{}_{j} + \mathcal{V}^{i}{}_{\hat{\nu}}\mathcal{V}^{\hat{\mu}}{}_{j}Y^{\hat{\nu}}{}_{\hat{\mu}}(\mathbf{x}) , \qquad (98)$$

where

$$Y^{\nu}{}_{\mu}(\mathbf{x}) = \sum_{k=1}^{\infty} \sum_{T\in\mathcal{T}^{\nu}{}_{\mu}(\mathbf{x},k)} W(T) .$$

From the fact that $\mathcal{V}^{i}{}_{B} = \mathcal{V}^{B}{}_{i} = 0$ for all $i \in B$, we see that the only nonzero contributions to Eq. (98) can come from terms of the form $\mathcal{V}^{i}{}_{\hat{l}}Y^{\hat{l}}{}_{\hat{k}}\mathcal{V}^{\hat{k}}{}_{j}$. From the inversion symmetry, we observe that

$$Y^{\hat{-l}}{}_{\hat{-k}} = Y^{\hat{l}}{}_{\hat{k}} .$$

Thus, Eq. (98) can be explicitly rewritten as

$$\tilde{J}^{i}{}_{j} = J^{i}{}_{j} + 2(X^{i\hat{+}}{}_{\hat{+}j}Y^{\hat{+}}{}_{\hat{+}} + X^{i\hat{-}}{}_{\hat{+}j}Y^{\hat{+}}{}_{\hat{-}}$$
$$+ X^{i\hat{0}}{}_{\hat{+}j}Y^{\hat{+}}{}_{\hat{0}} + X^{i\hat{+}}{}_{\hat{0}j}Y^{\hat{0}}{}_{\hat{+}}) + X^{i\hat{0}}{}_{\hat{0}j}Y^{\hat{0}}{}_{\hat{0}} ,$$

where

$$X^{i\hat{l}}{}_{\hat{k}j} = \mathcal{V}^{i}{}_{\hat{k}}\mathcal{V}^{\hat{l}}{}_{j} .$$

To evaluate $\tilde{\lambda}$, we need now only calculate the eigenvalues of q^{2}_{i} and q^{j}_{2} with respect to the matrices $X^{i\hat{l}}{}_{\hat{k}j}$ for each pair of values for l and k. Evaluating

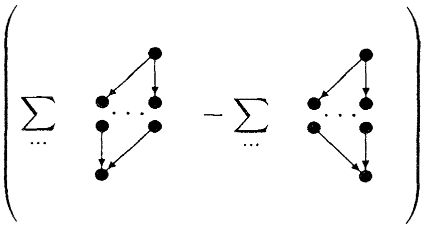
$$q^{2}_{i}\mathcal{V}^{i}{}_{\hat{+}} = -q^{2}_{i}\mathcal{V}^{i}{}_{\hat{-}} = 3p ,$$
$$\mathcal{V}^{\hat{+}}{}_{i}q^{i}_{2} = -\mathcal{V}^{\hat{-}}{}_{i}q^{i}_{2} = \tfrac{3}{2}pf(1-f) ,$$
$$q^{2}_{i}\mathcal{V}^{i}{}_{\hat{0}} = -\mathcal{V}^{\hat{0}}{}_{i}q^{i}_{2} = 0 ,$$

we have

$$\tilde{\lambda} = \lambda + 2q^{2}_{i}X^{i\hat{+}}{}_{\hat{+}j}q^{j}_{2}Y^{\hat{+}}{}_{\hat{+}} + 2q^{2}_{i}X^{i\hat{+}}{}_{\hat{-}j}q^{j}_{2}Y^{\hat{+}}{}_{\hat{-}}$$
$$= -3pf + 9p^{2}f(1-f)(Y^{\hat{+}}{}_{\hat{+}} - Y^{\hat{+}}{}_{\hat{-}}) . \qquad (99)$$

Diagrammatically, this equation can be expressed as

$$\tilde{\lambda} = -3pf + 9p^2 f(1-f)$$



, (100)

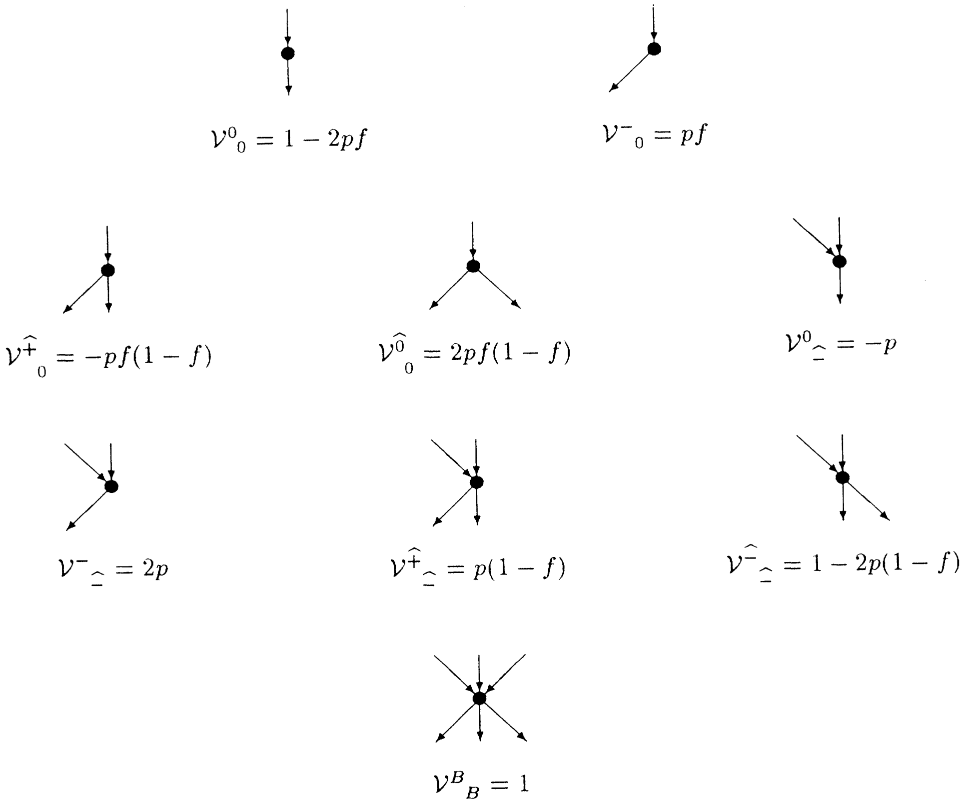


FIG. 5. Vertex factors for the 1D3P lattice gas.

where the notation in large parentheses indicates summation of the products of all internal vertex factors over all diagrams with the depicted initial and final configurations. Together, Eqs. (97) and (100), with vertices given in Fig. 5, constitute an *exact* expression for the diffusivity of the 1D3P lattice gas.

B. The Burgers equation lattice gas

Vertices

From either the collision operator or the state transition table for this lattice gas (see Sec. IV B) we can calculate the nonzero mean vertex coefficients, which are given by

$$V^B{}_B = V^{\varnothing}{}_{\varnothing} = 1, \quad V^+{}_{\pm} = \frac{1+a}{2},$$

$$V^+{}_B = -a, \quad V^-{}_{\pm} = \frac{1-a}{2},$$

$$V^-{}_B = a .$$

Using the equilibrium value f for the mean occupation numbers $N_0^{\pm}$, we can calculate the correlation vertex coefficients. Recall that we calculate the CVC's using only the zeroth-order mean occupation numbers. The CVC's are given by

$$\mathcal{V}^B{}_B = \mathcal{V}^{\varnothing}{}_{\varnothing} = 1, \quad \mathcal{V}^i{}_B = \mathcal{V}^B{}_j = 0 ,$$

$$\mathcal{V}^i{}_j = \tfrac{1}{2}, \quad \mathcal{V}^{\varnothing}{}_B = \mathcal{V}^B{}_{\varnothing} = 0 .$$

In particular, note that all the CVC's that modify the number of correlated quantities are zero. Thus, in this lattice gas, no $O(\epsilon)$ correlations are generated by gradients in N_1 and correlations cannot affect the hydrodynamic equation by influencing the single-particle means.

Because of the first-order collision operator Ω_1^i, which does not satisfy semidetailed balance, correlations might also be generated by the quantities $I^{\hat{\mu}}$. From Eq. (95), however, we have

$$I^B = 0 .$$

Thus we find that for this lattice gas, no correlations are generated to $O(\epsilon)$. Furthermore, even if correlations existed, they would not couple back to the hydrodynamic equations since $\mathcal{V}^{\pm}{}_B = 0$. It follows that the standard Chapman-Enskog analysis gives the correct results for the transport coefficients. In fact, a stronger version of this result has been proven using other methods [26].

C. 2D4P lattice gas

1. Vertices

Using the general formulas Eqs. (75) and (87) to calculate the correlation vertex coefficients $\mathcal{V}^{\alpha}{}_{\beta}$ for the 2D4P lattice gas, we arrive at the values for the CVC's that are depicted in Fig. 6. In this figure we have only included a single example of each equivalence class of vertices under the symmetry group generated by reflections across either axis. Furthermore, we have only included a single example of each pair of vertices that are related by a 90° rotation. The CVC's for such vertices are related by exchanging the two-particle densities $\mu\leftrightarrow\nu$. For example, we have

$$\mathcal{V}^{\bullet\!-}{}_{\bullet\!-} = 1 - 2\nu + 2\nu^2, \tag{101}$$

$$\mathcal{V}^{\overset{|}{\bullet}}{}_{\overset{|}{\bullet}} = 1 - 2\mu + 2\mu^2. \tag{102}$$

2. *Renormalization of eigenvalues*

Applying the theorems of Sec. VI G to the 2D4P lattice gas, we find that the renormalized J matrix must be of the form

$$\tilde{J}=\begin{bmatrix} \tilde{\lambda}^4/2 & 0 & -\tilde{\lambda}^4/2 & 0 \\ 0 & \tilde{\lambda}^3/2 & 0 & -\tilde{\lambda}^3/2 \\ -\tilde{\lambda}^4/2 & 0 & \tilde{\lambda}^4/2 & 0 \\ 0 & -\tilde{\lambda}^3/2 & 0 & \tilde{\lambda}^3/2 \end{bmatrix}.$$

The renormalized hydrodynamic equations are

$$\frac{\partial\mu}{\partial t}=\frac{\partial}{\partial x}\left[\tilde{\mathcal{D}}(\nu,\mu)\frac{\partial\mu}{\partial x}\right],$$

$$\frac{\partial\nu}{\partial t}=\frac{\partial}{\partial y}\left[\tilde{\mathcal{D}}(\mu,\nu)\frac{\partial\nu}{\partial y}\right],$$

with

$$\tilde{\mathcal{D}}(\mu,\nu)=\frac{c^2}{2\Delta t}\left[\frac{2}{(-\tilde{\lambda}^3)}-1\right]$$

and

$$\tilde{\mathcal{D}}(\nu,\mu)=\frac{c^2}{2\Delta t}\left[\frac{2}{(-\tilde{\lambda}^4)}-1\right].$$

In order to calculate the renormalized eigenvalue $\tilde{\lambda}^4$ it is

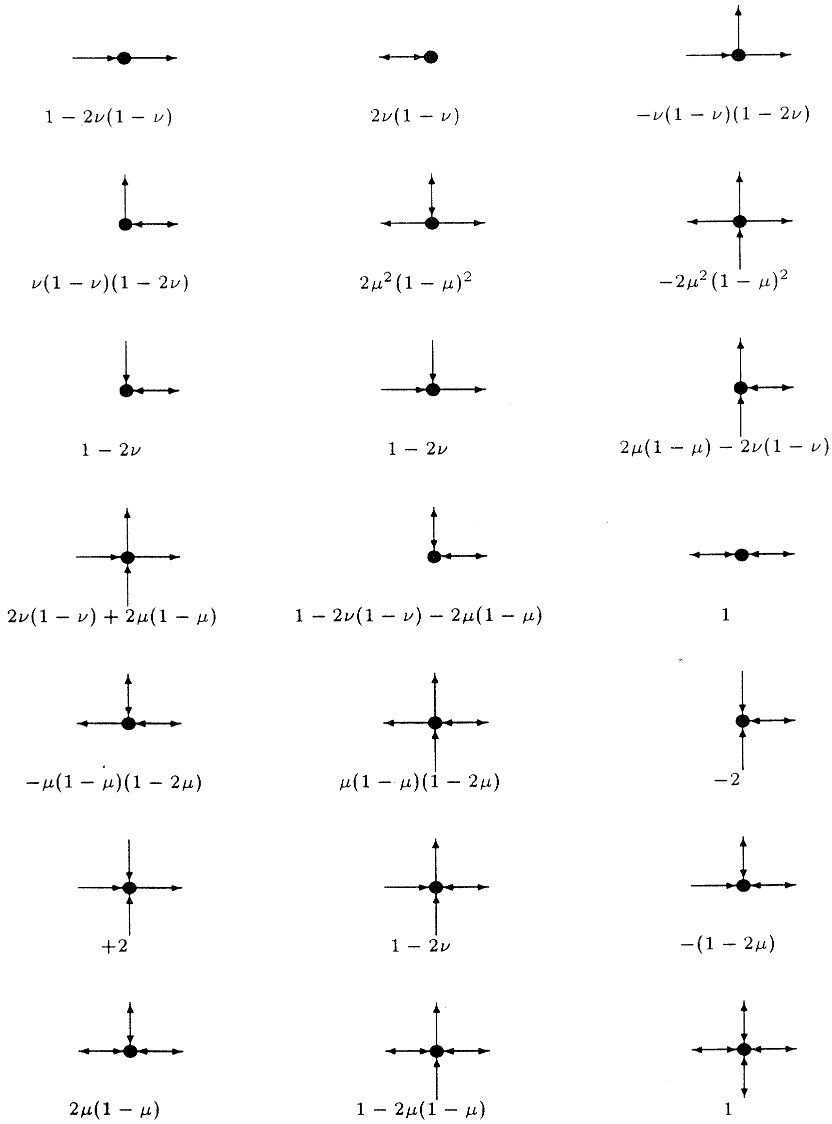


FIG. 6. Vertex factors for the 2D4P lattice gas.

only necessary to calculate the component $\tilde{J}^{1}{}_{1}$ of the renormalized J matrix. Because the lattice gas is invariant under the combination of a 90° rotation and the exchange $\mu \leftrightarrow \nu$, the eigenvalue $\tilde{\lambda}^3$ can be calculated from $\tilde{\lambda}^4$ by the exchange of particle densities.

Using a notation similar to that developed for the 1D3P lattice gas in Sec. VII A 2, we can write the renormalized matrix $\tilde{J}$ in the form of Eq. (98). Using the symmetry properties of the lattice gas to prove the equality of quantities $Y^{\alpha}{}_{\beta}$ which are related by reflections across each axis, we can simplify the expression for the shift in $\tilde{\lambda}^4$ to

$$\begin{aligned}\delta\lambda^4 = {}& 8\nu(\nu-1)(2\nu-1)^2\left[-Y^{\text{┗}}{}_{\text{┗}} + Y^{\text{┛}}{}_{\text{┗}} + Y^{\text{┓}}{}_{\text{┗}} - Y^{\text{┏}}{}_{\text{┗}}\right] + 16\nu^2(\nu-1)^2\left[Y^{\text{┣}}{}_{\text{┣}} - Y^{\text{┫}}{}_{\text{┣}}\right] \\ & +16\nu(\nu-1)(2\nu-1)\left[-Y^{\text{┣}}{}_{\text{┗}} + Y^{\text{┫}}{}_{\text{┗}}\right] + 16\nu^2(\nu-1)^2(2\nu-1)\left[Y^{\text{┗}}{}_{\text{┣}} - Y^{\text{┛}}{}_{\text{┣}}\right].\end{aligned}$$

Similarly, we have

$$\begin{aligned}\delta\lambda^3 = {}& 8\mu(\mu-1)(2\mu-1)^2\left[-Y^{\text{┏}}{}_{\text{┏}} + Y^{\text{┗}}{}_{\text{┏}} + Y^{\text{┛}}{}_{\text{┏}} - Y^{\text{┓}}{}_{\text{┏}}\right] + 16\mu^2(\mu-1)^2\left[Y^{\text{┳}}{}_{\text{┳}} - Y^{\text{┻}}{}_{\text{┳}}\right] \\ & +16\mu(\mu-1)(2\mu-1)\left[-Y^{\text{┳}}{}_{\text{┏}} + Y^{\text{┻}}{}_{\text{┏}}\right] + 16\mu^2(\mu-1)^2(2\mu-1)\left[Y^{\text{┏}}{}_{\text{┳}} - Y^{\text{┗}}{}_{\text{┳}}\right].\end{aligned}$$

These equations describe completely the renormalization of the hydrodynamic equations due to correlations. Each term $Y^{\alpha}{}_{\beta}$ corresponds to a set of diagrams with a specific set of outgoing and incoming virtual particles at the initial and final vertices of the diagram.

A rather dramatic simplification of the eigenvalue renormalization equations occurs when the equilibrium particle densities μ and ν are equal to $\frac{1}{2}$. When $\nu=\frac{1}{2}$, we have

$$\delta\lambda^4 = \left[Y^{\text{┣}}{}_{\text{┣}} - Y^{\text{┫}}{}_{\text{┣}}\right], \tag{103}$$

and when $\mu=\frac{1}{2}$ similarly

$$\delta\lambda^3 = \left[Y^{\text{┳}}{}_{\text{┳}} - Y^{\text{┻}}{}_{\text{┳}}\right]. \tag{104}$$

It follows that for these particular values of μ and ν, the set of diagrams that give a nonzero contribution to the renormalization of the eigenvalues is reduced to only those diagrams that have three outgoing virtual particles at the initial vertex and three incoming virtual particles at the final vertex. Thus, for example, the ring and two-particle BBGKY approximations for this lattice gas vanish at the equilibrium described by $\mu=\nu=\frac{1}{2}$.

In this particular case, the $\tau=3$ short-τ approximation is given by Eqs. (103) and (104), with the first Y term in each expression vanishing (because it is impossible to connect the outgoing and incoming particles in two time steps) and with the second arising from a single diagram of weight $\frac{1}{8}$. It follows that the corrected eigenvalues are equal to $-\frac{9}{8}$ in this simple approximation. This leads to $\tilde{\mathcal{D}}/\mathcal{D}=\frac{7}{9}=0.777\ldots$, which may be compared with the computer experimental value of $\mathcal{D}_{\text{expt}}/\mathcal{D}\approx 0.71$ [30].

In a future paper [38], we shall discuss in more detail the results of summing various subsets of diagrams for this lattice gas and compare the results to computer experimental data. The ring kinetic theory for this lattice gas has been worked out [31]; in this reference, a ringlike approximation is also used to treat noninteracting three-particle correlations, giving nonzero correction in the $\mu=\nu=\frac{1}{2}$ case.

D. FHP-I lattice gas

1. Vertices

Using the general formulas (75) and (87) to calculate the correlation vertex coefficients $\mathcal{V}^{\alpha}{}_{\beta}$ for the FHP-I lattice gas results in nearly 300 nonvanishing CVC's that are independent in the sense that they are not related by symmetries. While it is a straightforward task for a symbolic algebra computer program to compute and work with these quantities, it would not be useful to present all the results in this paper. Instead, Figs. 7, 8, and 9 present only the initial (one-to-many) vertices, the propagator (one-to-one) vertices, and the closure (many-to-one) vertices, respectively. These vertices are sufficient to compute all the diagrams in the kinetic ring approximation and in the $\tau=3$ short-τ approximation.

2. Renormalization of eigenvalues

The only transport coefficient of the FHP-I lattice gas that undergoes renormalization is the shear viscosity ν. From the general arguments in Sec. VI G, we see that the renormalized eigenvalues $\tilde{\lambda}^4$ and $\tilde{\lambda}^6$ must be equal, as they lie in a single irreducible representation of the symmetry group generated by a 60° rotation. In terms of these renormalized eigenvalues of the $\tilde{J}$ matrix, the renormalized shear viscosity $\tilde{\nu}$ is given by

$$\tilde{\nu}=\frac{c^2}{8\Delta t}\left[\frac{2}{(-\tilde{\lambda}^4)}-1\right].$$

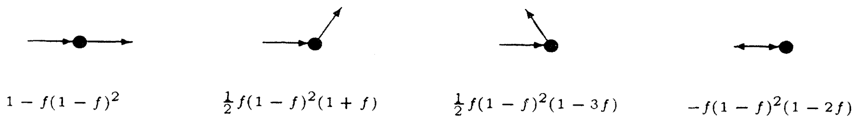


FIG. 7. Propagator vertex factors for the FHP-I lattice gas.

The renormalized eigenvalue $\tilde{\lambda}^4$ can be extracted from the $\tilde{J}$ matrix by taking the components

$$\tilde{\lambda}^4=6(\tilde{J}^1{}_1+\tilde{J}^1{}_2) .$$

As in the previous examples, we can express the eigenvalue shift in the form

$$\delta\lambda^4=6(X^{1\hat{\mu}}{}_{\hat{\nu}1}Y^{\hat{\nu}}{}_{\hat{\mu}}+X^{1\hat{\mu}}{}_{\hat{\nu}2}Y^{\hat{\nu}}{}_{\hat{\mu}}) .$$

By collecting coefficients of terms $Y^{\hat{\mu}}{}_{\hat{\nu}}$ that are related by symmetry, the expression for the eigenvalue shift reduces to a sum over more than 100 terms.

We shall not explore the diagrammatic expansion of the FHP-I lattice gas further in this paper. However, we have used the general expression for the renormalized shear viscosity to calculate several simple renormalization effects. In particular, one finds that in the ring approximation, the sum over diagrams diverges logarithmically; this result is well known for incompressible fluids in two dimensions and has been verified using other methods for the FHP-I lattice gas [23].

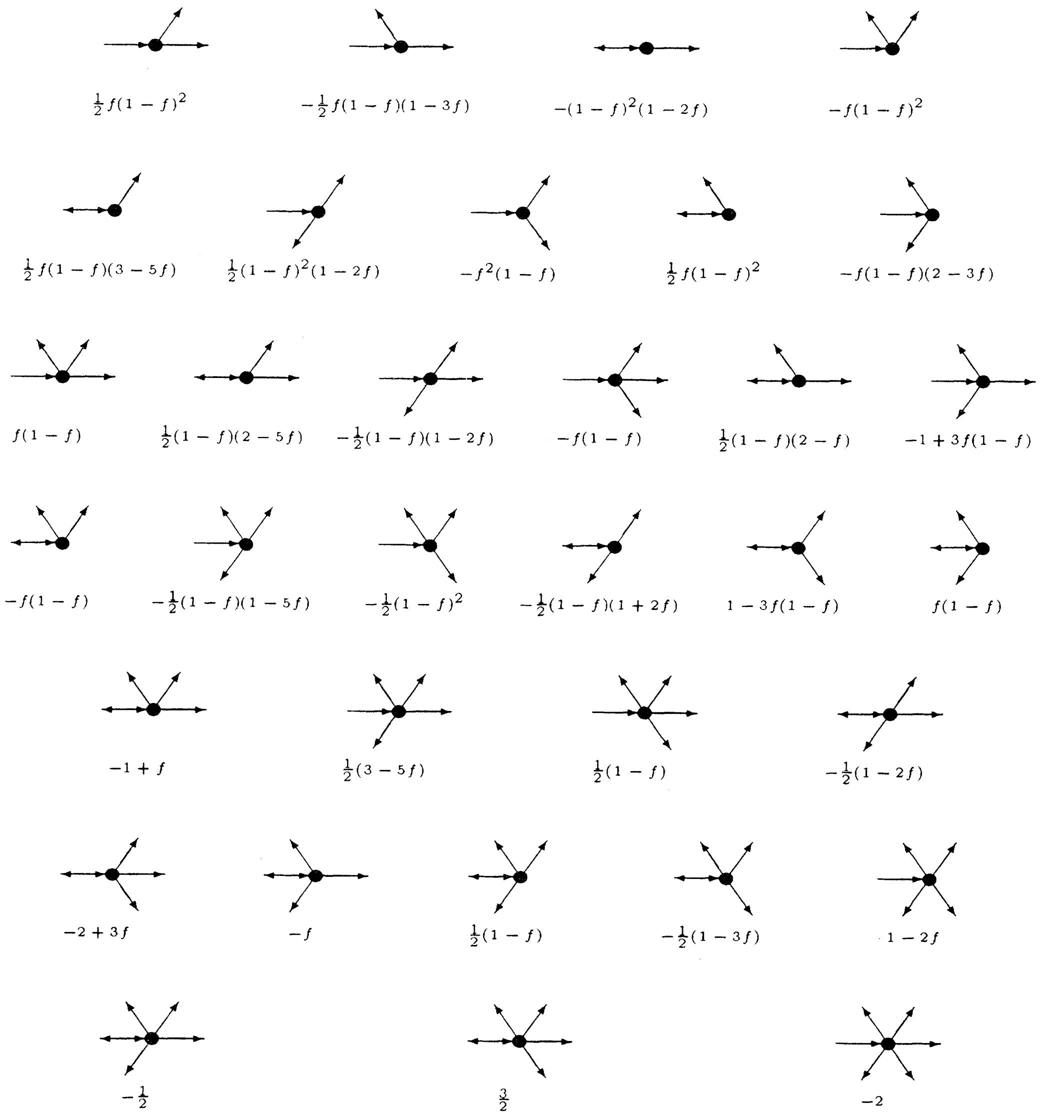


FIG. 8. Initial vertex factors for the FHP-I lattice gas.

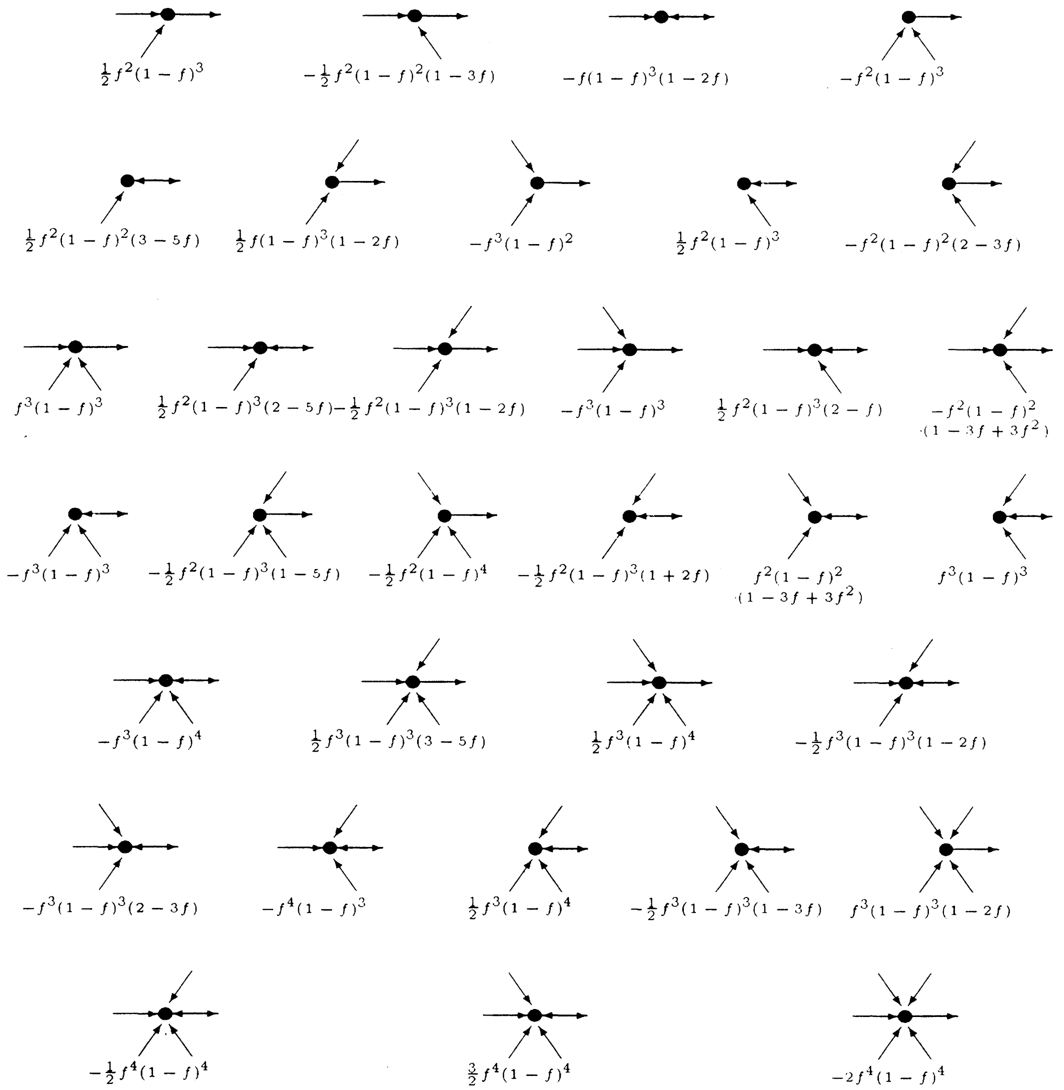


FIG. 9. Closure vertex factors for the FHP-I lattice gas.

VIII. APPROXIMATIONS AND NUMERICAL RESULTS FOR THE 1D3P LATTICE GAS

In this section we discuss in detail the sets of diagrams for the 1D3P lattice gas that correspond to the various approximation methods described in Sec. VI G and perform the associated partial diagrammatic sums. The goal of this detailed analysis is to use the simple 1D3P lattice gas as a test case to study the relative accuracy of the different approximations and the relative difficulty of computing these approximations. The results for this lattice gas hopefully give a good indication of what approaches will lead to useful results for more complicated lattice gases.

Correlations cause corrections to the Boltzmann diffusivity of the 1D3P lattice gas that are as large as 5% for certain values of the particle density f and bounce probability p. We describe in this section the results of numerical calculations of the partial diagrammatic sums corresponding to the various approximation methods and compare to empirical results from computer simulations of this lattice gas. In Sec. VIII A we calculate corrections to the diffusivity in the short-τ approximation. By graphing these corrections and comparing to computer experiment, we see that as τ increases these approximations give corrections to the Boltzmann approximation that seem to converge to the observed values. The convergence is slow, however, and since the calculation of these corrections is computationally quite expensive, it is difficult to estimate the asymptotic value of the diffusivity to a high degree of accuracy using these approximations. In Sec. VIII B we apply the partial BBGKY summation prescription and again graph the results compared to computer experimental values. For small values of k, the k-particle BBGKY diagrammatic summation converges rapidly, and in most ranges for which we have calculated the results, these approximations approach monotonically the computer experimental values as k increases. In this subsection we also include a proof that the two-particle BBGKY approximation converges for arbitrary values of $p,f>0$. In Sec. VIII C we observe that in the vicinity of the density value $f=1$, the corrections to the Boltzmann approximation can be expanded in a power series in the variable $\varepsilon=1-f$. The diagrams that contribute corrections of order ε^n are the diagrams that have n or fewer vertices where a single virtual particle branches out to two virtual particles ("1-2" vertices). This expansion in ε is roughly equivalent to the familiar expansion in the continuum theory or in quantum field theory in terms of the number of loops. Using this expansion, we can numerically evaluate the successive derivatives of the correction term at $f=1$ and compare these results to computer experiment. The corrections thus calculated agree exactly with our computer experimental results to within the statistical accuracy of those results. This calculation has the additional feature that it is possible to prove that the sum over all diagrams that contribute to a given order in ε converges. This convergence follows from the fact that the sum over all diagrams that contain a fixed number of 1-2 vertices is convergent; we prove this for the case of a single 1-2 vertex using an argument that can be generalized in a straightforward fashion. In Sec. VIII D we consider the ring approximation from an analytic perspective and compare this approximation to the closely related two-particle BBGKY approximation. Finally, in Sec. VIII E we briefly compare the results of the varied approximation methods used in this section.

A. Short-τ approximation

Consider the corrections to the eigenvalue λ in the Chapman-Enskog analysis of the 1D3P lattice gas arising from diagrams of fixed length τ. The first few such corrections are easy to evaluate by hand. For $\tau=3$, the only diagrams contributing to Eq. (99) are the two diagrams T_1 and T_2 shown in Fig. 4. These two diagrams shift the eigenvalue λ by

$$\begin{aligned}\delta\lambda=\tilde{\lambda}^{(3)}-\lambda&=9p^2f(1-f)[(fp)^2-fp(1-2fp)]\\&=-9p^3f^2(1-f)(1-3fp)\ ,\end{aligned}\tag{105}$$

where we denote by $\tilde{\lambda}^{(3)}$ the eigenvalue of q_i^2 in the $\tau=3$ matrix $\tilde{J}^{(3)i}{}_j$. For $\tau=4$, there are 22 diagrams that contribute to Eq. (99). The 11 diagrams contributing to $Y^{\hat{+}}{}_{\hat{+}}$ are shown in Fig. 10; the diagrams contributing to $Y^{\hat{+}}{}_{\hat{-}}$ can be generated from these by simply changing the directions of the initial pair of virtual particles. The correction to λ for $\tau=4$ is given by

$$\begin{aligned}\delta\lambda&=\tilde{\lambda}^{(4)}-\tilde{\lambda}^{(3)}\\&=9p^4f^2(1-f)(1-3fp)(4-3f-3f^2p)\ .\end{aligned}\tag{106}$$

The complete correction in the $\tau=4$ short-τ approximation is given by summing the shifts in Eqs. (105) and (106). As τ increases, the number of diagrams contributing to $\delta\lambda$ increases exponentially and it rapidly becomes impractical to compute the exact correction, even using numerical computing techniques, without some means of simplifying or approximating the calculation. We have calculated the corrections to λ including diagrams up to $\tau=5$. The resulting short-τ approximations $\tilde{\lambda}^{(\tau)}$ are plotted against f and compared to computer experiment for $p=\frac{1}{4}$ and $\frac{1}{2}$ in Figs. 11 and 12, respectively. Although the results of this calculation are a great improvement over the Boltzmann approximation and clearly appear to be converging to the computer experimental values as τ increases, the oscillatory nature of these approximations (in τ) is an undesirable feature that makes it difficult to use partial results to put bounds on the actual diffusivity. Nonetheless, it is clear from the graphs in Figs. 11 and 12 that this formalism includes empirically measurable effects that are completely dropped in the Boltzmann approximation.

B. BBGKY approximations

We now consider the partial BBGKY approximations for the 1D3P lattice gas. As described in Sec. VI, the k-particle BBGKY approximation is given by summing over all diagrams that have at most k simultaneously correlated virtual particles. For each k, the approximation thus consists of an infinite number of diagrams. This approximation can be reduced to a finite sum by also limiting the lengths of the diagrams to some maximum size τ as in the short-τ approximation. Because for fixed k the computational complexity of the summation of graphs of length less than or equal to τ grows polynomially in τ rather than exponentially as in the short-τ approximation, it is easier to compute the limit of the set of k-particle diagrams as $\tau\rightarrow\infty$ than the complete set of diagrams in this limit. For $k=2$, it is possible to prove that this infinite sum of diagrams must in fact converge; we derive this result later in this subsection. For $k>2$, we do not have a complete proof of convergence; however, numerical evidence indicates that for each k, the infinite k-particle BBGKY sum of diagrams is convergent. By using methods like those used in the following subsection, it may be possible to prove that for each k, the BBGKY approximation converges.

We have used a computer to numerically calculate the limit of the full k-particle BBGKY approximation for certain values of f and p. The algorithm we used was to sum all diagrams of length less than or equal to τ on a lattice of width l and then to take the limits as $\tau,l\rightarrow\infty$. As an example, for a characteristic pair of values $(p,f)=(0.25,0.5)$, we have graphed in Fig. 13 the corrections due to two-particle BBGKY diagrams of length less than or equal to τ on a lattice of size l for all $\tau<30$ and for lattice sizes 2, 3, 4, 8, and 16. The curve for $l=8$ is indistinguishable from, and hidden by, the curve for $l=16$. Note that all diagrams of length τ are correctly summed as long as $l\geq\tau$ for all k; for $k=2$, however, many diagrams cancel so that larger values of τ give correct results, such as for $l=2$, $\tau=4$. It is clear from this graph not only that the sum over diagrams converges rapidly, but also that the major part of the sum arises from the contributions of diagrams that are of lim-

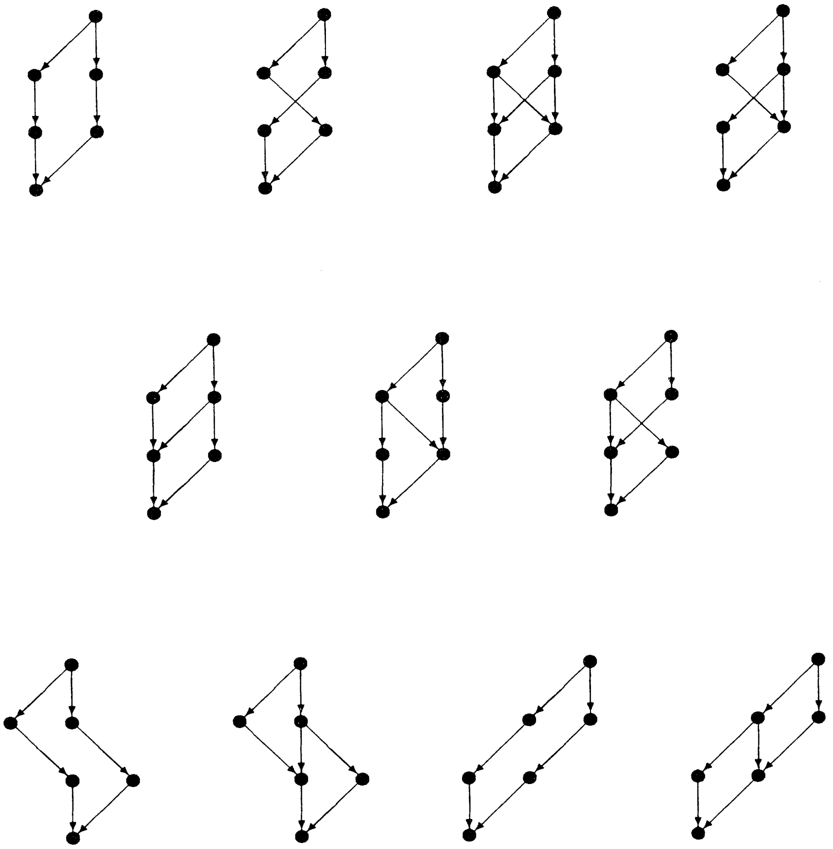


FIG. 10. Diagrams contributing to the $\tau=4$ correction for the 1D3P lattice gas.

ited width. We have numerically approximated the limits of the k-particle BBGKY sums for $k \leq 5$. The results of this calculation are graphed in Figs. 14 and 15 for the same ranges of values for p,f that were used for the short-τ approximations in Figs. 11 and 12.

We conclude this subsection with a proof that the two-particle BBGKY approximation is convergent. Although this proof is carried out for the particular 1D3P lattice gas, it generalizes easily to other systems. We begin by considering a matrix M on the space B_2 of two-particle subsets of B. The matrix element $M^{\hat{i}}{}_{\hat{j}}$ is defined by summing over all two-particle diagrams that begin with outgoing VP's $\hat{j}$ at an initial vertex and conclude with incoming VP's $\hat{i}$ at a final vertex and that have the property that all internal vertices have a single incoming and outgoing VP. In particular, this means that not only are we restricting to two-particle diagrams, but we are also selecting that subset of diagrams that have no interaction vertices other than the initial and final points. Because the internal vertices $\mathcal{V}^{i}{}_{j}$ describing propagation of a single correlated quantity are symmetric in i and j and satisfy the conditions

$$0 \leq \mathcal{V}^{i}{}_{j} \leq 1$$

and

$$\sum_{i} \mathcal{V}^{i}{}_{j} = \sum_{i} \mathcal{V}^{j}{}_{i} = 1 \ , \qquad (107)$$

it is fairly straightforward to see that the matrix elements of M must satisfy the same constraints. Intuitively, the above conditions on $\mathcal{V}^{i}{}_{j}$ can be interpreted as arising from a description of the propagation of a single correlated quantity as a discrete random walk, where the direction of the walk at a given time is dependent on the direction of the walk at the previous time step, according to the rule that the (virtual) particle will change direction with probability $g=fp$ and will continue moving in the same direction with probability $1-2g$. The possible directions of the walk correspond to the lattice vectors $\mathbf{e}_0, \mathbf{e}_{\pm}$. With this interpretation, the matrix element $M^{\hat{i}}{}_{\hat{j}}$ gives the probability that a pair of virtual particles that begin in state $\hat{j}$ will collide for the first time in state $\hat{i}$. Because for $g>0$ the probability is 1 that two particles beginning at the same lattice site will eventually collide, it follows that condition (107) must hold for the matrix M. The remaining conditions on M of symmetry and positivity follow immediately from the random-walk interpretation.

It is now possible to give a complete description of the two-particle BBGKY approximation in terms of the matrix M. The two-particle BBGKY correction to the transport coefficients of any lattice gas can be described in terms of the correction to the J matrix

$$\delta J^{i}{}_{j} = \mathcal{V}^{i}{}_{lm} \overline{M}^{lm}{}_{np} \mathcal{V}^{np}{}_{j} \ ,$$

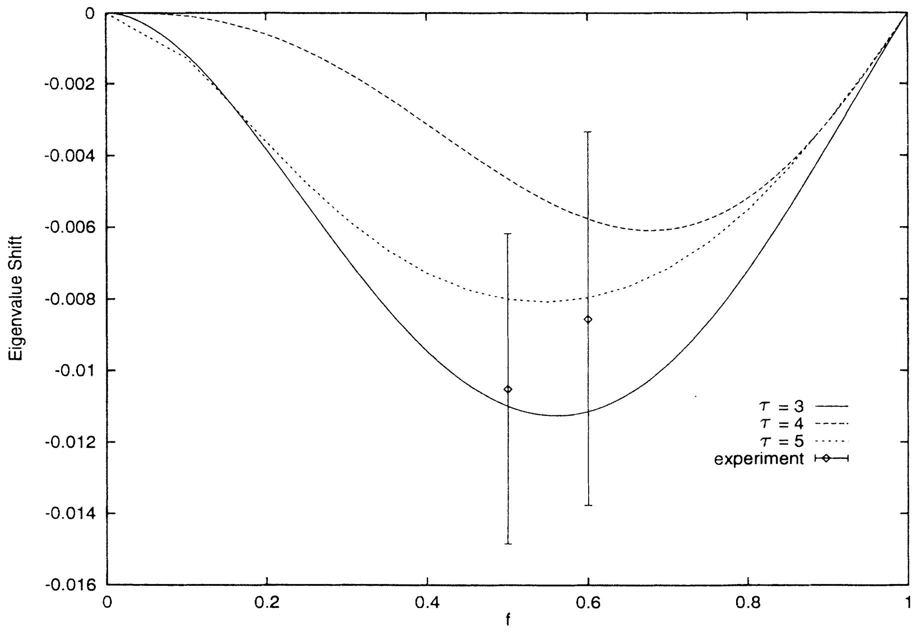


FIG. 11. Short-τ approximations for $p=\frac{1}{4}$.

where $\overline{M}$ is a matrix in the space B_2 defined by summing over all two-particle diagrams. This matrix is defined in a similar fashion to M; however, now we are including diagrams that have an arbitrary number of two-particle interaction vertices $\mathcal{V}^{\hat{i}}{}_{\hat{j}}$. By considering these two-particle interactions as another matrix $\mathcal{V}$ in the space B_2, we can write a matrix equation for $\overline{M}$ in terms of M and $\mathcal{V}$,

$$\overline{M}=M+M\mathcal{V}\overline{M} \ .$$

Formally, this equation has the solution

$$\overline{M}=M(1-\mathcal{V}M)^{-1} \ . \tag{108}$$

The matrix $\mathcal{V}$ restricted to the space B_2 is easily seen to be another positive definite symmetric matrix that satisfies Eq. (107). It follows that the matrix $\mathcal{V}M$ has the same properties. Unfortunately, this appears to lead to a difficulty, namely, it is a consequence of Eq. (107) that all these matrices have an eigenvalue of 1, with associated eigenvector (1,1,1). This means that the matrix $1-\mathcal{V}M$ has a 0 eigenvalue and thus has no inverse. However, we are not interested in computing the complete matrix $\overline{M}$. Rather, we are interested in computing the part of that matrix that contributes to the renormalization of the eigenvalue λ. The correction to this eigenvalue due to the

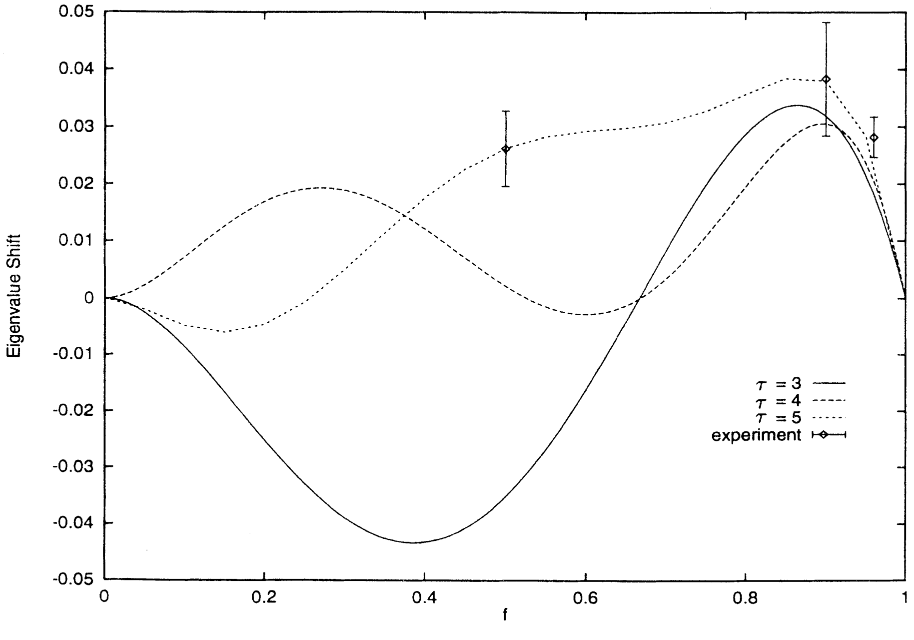


FIG. 12. Short-τ approximation for $p=\frac{1}{2}$.

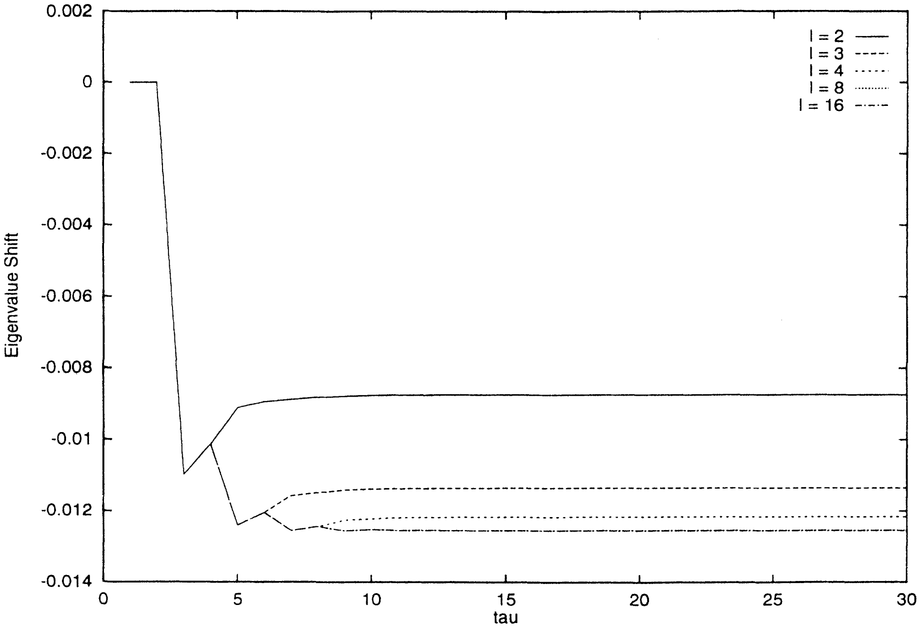


FIG. 13. Two-particle BBGKY corrections for $(p,f)=(\frac{1}{4},\frac{1}{2})$.

two-particle BBGKY approximation is given by

$$\delta\lambda=9p^2f(1-f)[\overline{M}^{\hat{+}}{}_{\hat{+}}-\overline{M}^{\hat{-}}{}_{\hat{+}}] . \tag{109}$$

The quantity in square brackets can be rewritten in matrix form as

$$q^2\overline{M}q_2=q^2(M+M\mathcal{V}M+M\mathcal{V}M\mathcal{V}M+\cdots)q_2 ,$$

where in the basis $(\hat{+},\hat{0},\hat{-})$, $q^2=(-1,0,+1)$ is the usual left eigenvector of the J matrix and q_2 is the corresponding right eigenvector. By the same symmetry arguments that we used in Sec. VI G to prove that the vectors q^i are eigenvectors of the renormalized J matrix, it follows that q^2 must be an eigenvector of M with some eigenvalue l. Similarly, q^2 is an eigenvector of $\mathcal{V}$ (considered as a matrix in the space B_2). It is straightforward to verify from the vertex rules that the eigenvalue of q^2 in this matrix is $1-3p+3pf$. Thus, due to the fact that q^2 is orthogonal to the eigenvector (1,1,1), we avoid the divergence associated with the unit eigenvalue of this vector. In terms of the eigenvalue l it is possible to rewrite Eq. (109) in the form

$$\delta\lambda=9\frac{p^2f(1-f)l}{1-l(1-3p+3pf)} , \tag{110}$$

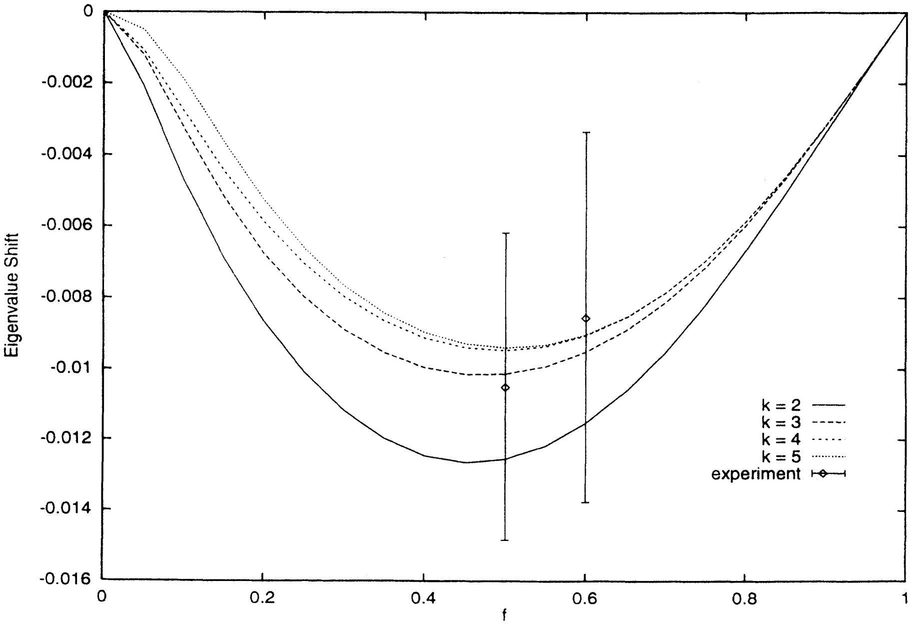


FIG. 14. Partial BBGKY approximations for $p=\frac{1}{4}$.

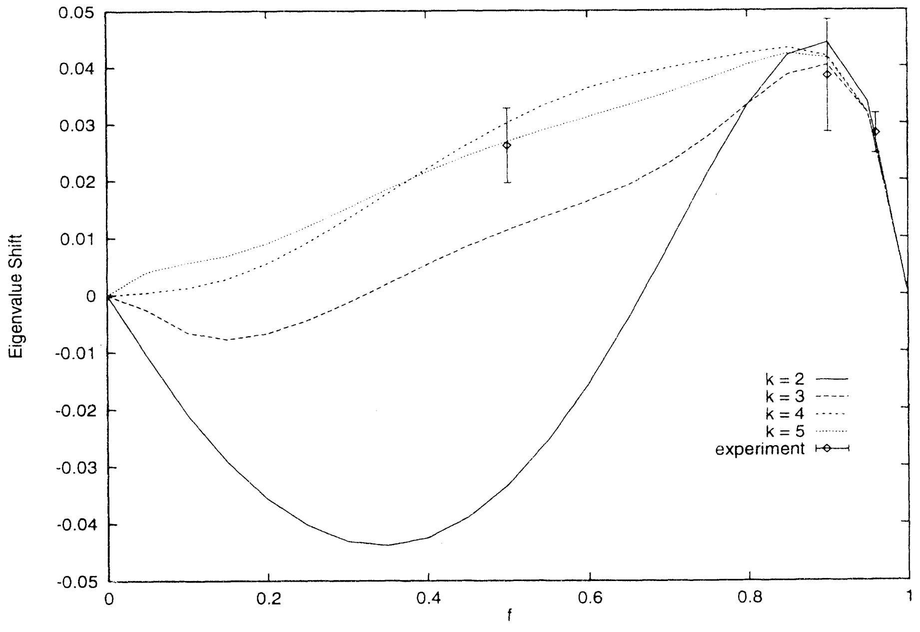


FIG. 15. Partial BBGKY approximations for $p=\frac{1}{2}$.

which is manifestly a finite renormalization. We have thus shown that for the 1D3P lattice gas, the two-particle BBGKY correction is finite for any p,f. To check this result, we have numerically estimated the matrix M for certain values of p,f and verified that Eq. (110) gives a correction that agrees with the numerical results obtained from the general BBGKY computer code described above. As an example, for $(p,f)=(0.25,0.5)$ we get a matrix M, which is approximately

$$M\approx\begin{bmatrix}0.305\,894 & 0.293\,698 & 0.400\,407\\ 0.297\,612 & 0.404\,777 & 0.297\,612\\ 0.400\,407 & 0.293\,698 & 0.305\,894\end{bmatrix} .$$

The eigenvalue of q^2 for this matrix is $l=-0.094\,513$. The estimated two-particle BBGKY correction to the eigenvalue λ is thus

$$\delta\lambda=\frac{9l}{64-40l}\approx-0.012\,550 ,$$

in excellent agreement with the results computed numerically and graphed in Fig. 13.

A particularly simple example of this formalism arises in the case $g=fp=\frac{1}{3}$. In this case, the random walk in terms of which M is described is a true random walk, with the probability at each time step of each of the three possible directions being exactly $\frac{1}{3}$, independent of the direction of the previous step. It follows immediately from a consideration of the matrix M that the eigenvalue l of q^2 is in this case 0, which implies that the shift to the diffusivity arising from the two-particle BBGKY approximation is 0 whenever $g=\frac{1}{3}$. Note, however, that the higher-k BBGKY approximations do *not* generally vanish in this case. For example, in Fig. 15 the two-particle BBGKY approximation vanishes at the point $(p,f)=(\frac{1}{2},\frac{2}{3})$; however, the higher-$k$ approximations do not vanish and are closer to the computer experimental results.

C. Expansion around $f=1$

In this subsection we consider the renormalization of λ when the particle density f approaches 1. In this regime, it is possible to expand the eigenvalue $\tilde{\lambda}$, and thus the diffusivity, in the quantity $\varepsilon\equiv 1-f$. By rewriting the correlation vertex coefficients in terms of ε, we can ascertain which diagrams contribute to each order in ε. The CVC's are shown in terms of ε and $g=fp$ in Fig. 16. Note that both vertices that take a single incoming virtual particle to two virtual particles (1-2 vertices) are proportional to ε. Since these vertices are the only nonzero vertices that increase the number of virtual particles in a diagram, it follows that the set of diagrams that contributes to order ε^n must be a subset of the diagrams in the $(n+1)$-particle BBGKY approximation. In fact, aside from the interactions described by the vertices with two and three virtual particles in both the incoming and outgoing states, the ordering of diagrams in ε is equivalent to the loop ordering of diagrams that is commonly used in continuum kinetic theory and quantum field theory. Because the sets of diagrams that contribute to the corrections for low orders in ε are fairly simple (but infinite), we can numerically evaluate these partial diagrammatic sums to get a prediction for the low-order derivatives of the diffusivity D around $f=1$. Because the factor g appears in the 1-1 vertices $\mathcal{V}^i{}_j$, it is convenient to fix this quantity while evaluating the derivatives of D with respect to ε. The numerical calculation of the low-order coefficients as a sum over diagrams converges quite rapidly. In fact, it can be shown that for each n, the coefficient of ε^n gives a convergent sum; we outline a proof of this fact at the end of this subsection.

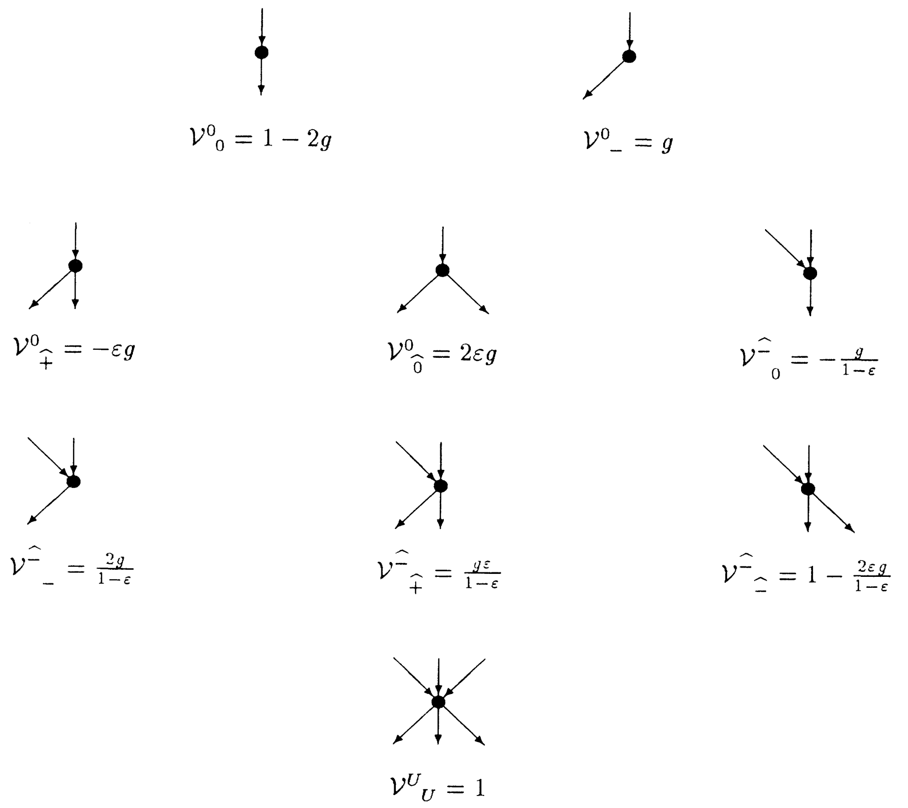


FIG. 16. Correlation vertex coefficients in terms of g, ε.

As the simplest example of this type of calculation, consider the set of diagrams that contribute to order ε in $\tilde{\lambda}$. Because the correction factor in Eq. (100) is itself proportional to ε, the diagrams that contribute linearly in ε cannot contain any internal 1-2 vertices; the contribution to the eigenvalue from such diagrams is equivalent to the two-particle BBGKY contribution using the limits of the 2-2 vertices as $\varepsilon \to 0$. Using the results of Sec. VIII B, this contribution is finite and can be computed just as the two-particle BBGKY correction is calculated above. As an example, consider again the case where $g = \frac{1}{3}$. In this case, we expect the derivative of $\tilde{\lambda}$ at $f = 1$ to be 0; this result seems to be in agreement with computer experiment.

We have numerically calculated the first three derivatives of $\tilde{\lambda}$ at the point $f = 1$ for several values of the parameter g. The results are completely in agreement with computer experimental results when $1 - f \ll 1$. As an example, we have graphed the quadratic and cubic approximations to $\delta\lambda = \tilde{\lambda} - \lambda$ for $g = 0.48$ in Fig. 17 and compared to computer experimental data at the point $f = 0.96$. For comparison, the curves describing the $\tau = 3$ and 4 short-τ approximations are also graphed in this region. Note that the region of the graph with $f < 0.96$ corresponds to $p > \frac{1}{2}$ and is unphysical.

We conclude this subsection with an outline of the proof that the sum over diagrams contributing to the ε^n term in $\tilde{\lambda}$ is convergent for any fixed value of n. This proof is similar in nature to the proof of convergence for the two-particle BBGKY approximation in Sec. VIII B, but is slightly more subtle. As mentioned above, to prove the desired result it will suffice to show that the contribution from all diagrams with n vertices of the 1-2 type gives a convergent sum for all values of n. As the simplest example beyond the two-particle BBGKY approximation, we consider the contribution to the order ε^2 term arising from diagrams with a single internal 1-2 vertex. Using an analogous notation to that used in Sec. VIII B for the analysis of the two-particle BBGKY approximation, the contribution from the diagrams with a single internal 1-2 vertex can be written as

$$\delta\lambda = 9p^2 f(1-f)(\overline{M}{}^{\hat{+}}{}_{\hat{+}} - \overline{M}{}^{\widehat{\;}}{}_{\hat{+}}) ,$$

where $\overline{M}$ is given by

$$\overline{M}{}^{\hat{i}}{}_{\hat{j}} = [(1 - M\mathcal{V})^{-1}]^{\hat{i}}{}_{\hat{k}} M^{\hat{k}}{}_x \mathcal{V}^x{}_y M^y{}_z [(1 - \mathcal{V}M)^{-1}]^z{}_v \times \mathcal{V}^v{}_w M^w{}_{\hat{m}} [(1 - \mathcal{V}M)^{-1}]^{\hat{m}}{}_{\hat{j}} . \tag{111}$$

In this equation, the variables x and w are summed over all distinct elements of the set of pairs of bits at distinct lattice points, modded out by equivalence under translation. The elements of this set $B_{1,1}$ are in a one-to-one correspondence with triplets (n,i,j), with $n > 0$ giving the distance between the lattice points of the two bits and i,j denoting the elements of the set B corresponding to the two bits. The variables y, z, and v are similarly summed over all elements of the set $B_{1,2}$ of triplets $(n,i,\hat{j})$ representing a single bit i at a distance n from a pair of bits $\hat{j} \in B_2$. This set contains elements with n both positive and negative since the lattice point with a

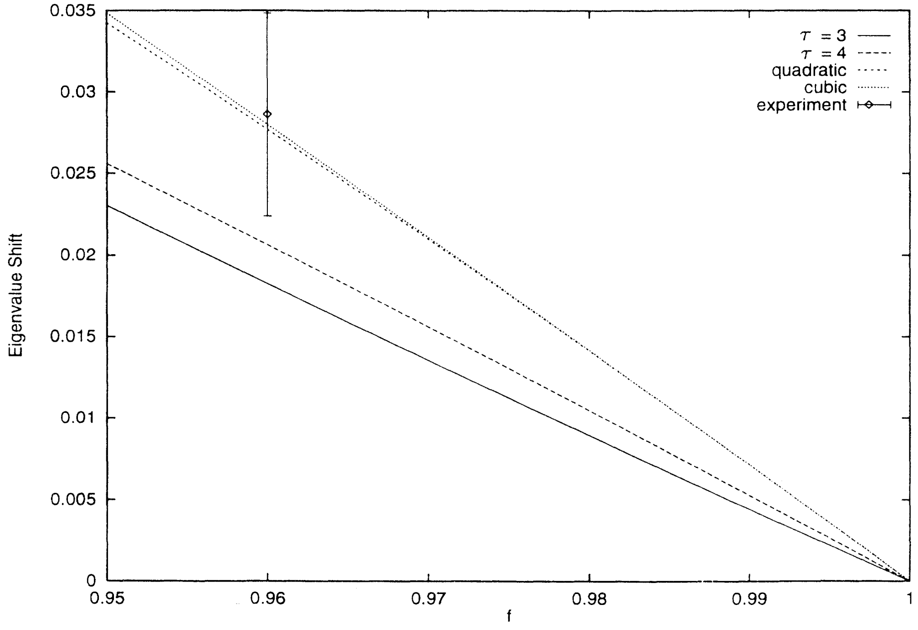


FIG. 17. Quadratic and cubic approximations to $\tilde{\lambda}^2$ around $f=1$ for $g=fp=0.48$.

single VP can be on either side of the lattice point with two VP's; there is a single element of the set $B_{1,2}$ with $n=0$ corresponding to the situation where all three particles are at the same lattice site. With this constraint on the summation variables, the matrices M and $\mathcal{V}$ are defined in an analogous fashion to the two-particle BBGKY case. For example, the matrix $M^y{}_z$ is the matrix on the space $B_{1,2}$ whose entries correspond to the probability that a set of three particles beginning in state z will first have a collision when they are in the state y. Similarly, the matrix $M^{\hat{k}}{}_x$ gives the sum over all two-particle diagrams with no (internal) collisions that begin in the state described by x and end with the collision described by the state $\hat{k}$. The matrix $\mathcal{V}^x{}_y$ always describes the product of correlation vertex coefficients involved in a collision from a state y to a state x; when both y and x are in $B_{1,2}$, we insist that the two particles remain at the same lattice site. Note that if a collision involves virtual particles at more than one lattice point, the distances between the vertices must be commensurate in both states for this matrix element to be nonzero. In Eq. (111), the matrix inverses of the form $(1-x)^{-1}$ should be taken to be shorthand for the formal expansion $\sum_i x^i$, as these matrices generally have a unit eigenvalue. Just as in the BBGKY case, it is straightforward to verify that all matrices considered here that are square (have both indices taking values in the same space) are symmetric, nonnegative, and satisfy condition (107). Equation (111) can be sketched diagrammatically as in Fig. 18.

By noting that $\overline{M}$ and its expression (111) are symmetric, an argument identical to that in Sec. VIII B tells us that the contribution to the eigenvalue λ can be described by the matrix formula

$$\delta\lambda = 9\frac{p^2 f(1-f)l^2}{[1-l(1-3p+3pf)]^2} \times q_k^2\{M^{\hat{k}}{}_x \mathcal{V}^x{}_y M^y{}_z[(1-\mathcal{V}M)^{-1}]^z{}_v \mathcal{V}^v{}_w M^w{}_{\hat{m}}\}q_2^m \,. \tag{112}$$

We have thus reduced the problem of proving that Eq. (111) is convergent to the problem of proving convergence for Eq. (112). There are several key arguments necessary to proving the convergence of this remaining sum. The first step is to prove that any matrix element of the form

$$\hat{M}^x{}_w = \mathcal{V}^x{}_y M^y{}_z[(1-\mathcal{V}M)^{-1}]^z{}_v \mathcal{V}^v{}_w$$

is convergent and has an absolute value bounded above by some number Ξ. The second step is to argue that the infinite sum

$$\sum_{w\in B_{1,1}} M^w{}_{\hat{m}} \tag{113}$$

converges for all $\hat{m}$ and thus can be bounded above by another number Δ. Once these two facts are shown, it follows immediately that the total eigenvalue shift is bounded above by

$$|\delta\lambda| < 9\frac{p^2 f(1-f)l^2}{[1-l(1-3p+3pf)]^2}\Xi\Delta^2 \,.$$

We shall now proceed to prove these two necessary convergence results. We first show that there is an upper bound Ξ on the matrix elements $\hat{M}^x{}_w$. For a fixed value of x, the matrix elements $\mathcal{V}^x{}_y$ form a vector in $B_{1,2}$,

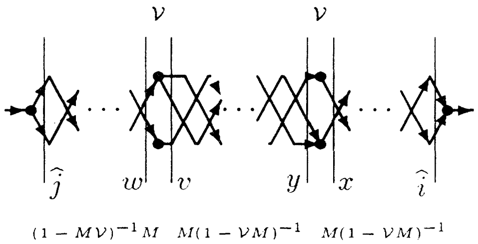


FIG. 18. Diagrammatic sketch of Eq. (111).

which we shall refer to as t_y. An examination of the collision rules (96) tells us that t has only eighteen nonzero components: eight of magnitude $-g^2\varepsilon$, four of magnitude $2g^2\varepsilon$, four of magnitude $-g(1-2g)\varepsilon$, and two of magnitude $2g(1-2g)\varepsilon$. We shall now consider the result s of multiplying this vector by the matrix M

$$s_z = t_y M^y{}_z \ .$$

Because the sum of the components of t is 0, the same must be true of the vector s. Furthermore, if we define a norm on t by

$$|t| = \sum_y |t_y| \ ,$$

then we can proceed to show that

$$|s| \le |t|[1-g^6(1-2g)^2] \ . \tag{114}$$

This result follows because there is always at least one set of diagrams of order $g^6(1-2g)^2$ that cancel between the positive and negative elements of t (in practice, much cancellation occurs; however, we are interested here only in the convergence). An example of three diagrams giving such a cancellation is given in Fig. 19. The vertex factors from these diagrams are identical; however, the diagrams connect to components of t_y with opposite sign. We do not depict the motion of the extra particle, which can be assumed to be constant for the three diagrams. From Eq. (114), it follows that every matrix element of $\hat{M}$ is bounded above by

$$|\hat{M}^x{}_w| \le \Xi = \frac{24pg\varepsilon}{g^6(1-2g)^2} \ .$$

Thus we have an upper bound of the desired form for the matrix elements of $\hat{M}$.

Finally, it remains to demonstrate that the infinite sum (113) is bounded above for all $\hat{m}$. This sum, however, is simply equal to the expected value of the number of time steps necessary for a pair of random walks beginning in state $\hat{m}$ to collide. To see this, observe that every diagram with weight $W(T)$ containing two noncolliding random walks that contributes to $M^{\hat{i}}{}_{\hat{m}}$ will contribute to the sum (113) a total of $\tau W(T)$, where τ is the length of the diagram; the factor τ appears because the diagram can be chopped in half at any point x and will contribute a factor of $W(T)$ for each such division. Given this interpretation, however, it is clear that the sum is convergent due to the standard result that in one dimension a random walk will return to any point on the lattice in a finite expected time (this result is usually stated for random walks without memory; however, a generalization to random walks with memory and nonzero bounce probability is straightforward). In conclusion, we have proven both convergence bounds that were needed to demonstrate conclusively the convergence of the sum over diagrams that contain a single 1-2 vertex. This implies the convergence of the order ε^2 term in the diffusivity around $f=1$. It is fairly straightforward to generalize these arguments to the coefficient of an arbitrary order ε^n by showing that the sum over diagrams with any fixed number of 1-2 vertices is convergent; however, the details become correspondingly more complex and are left as an exercise to the reader. Note also that we do not have any reason other than empirical results to believe that the expansion of $\tilde{\lambda}$ in ε has a nonzero radius of convergence, even though the coefficients themselves are proven to be finite.

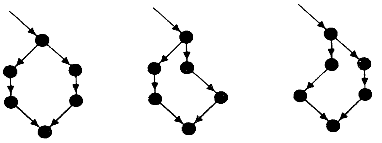


FIG. 19. Canceling diagrams.

D. Ring approximation

We now consider the ring approximation for the 1D3P lattice gas. In this subsection we study the ring approximation from two perspectives. First, we show that the ring approximation can be formulated in terms of the M matrix in the same form as the two-particle BBGKY approximation, where the collision matrix $\mathcal{V}$ is replaced by a new effective collision matrix. This formalism gives an analytic relationship between the corrections to λ from the ring approximation and the two-particle BBGKY approximation. Second, we perform an explicit analysis of the ring approximation in Fourier space and describe the complete contribution to the eigenvalue renormalization from this approximation.

The ring approximation is taken by summing over all independent paths for two separate virtual particles to propagate from one point to another, using for each virtual particle the 1-1 CVC's as weights on the vertices of the independent paths. The set of diagrams associated with this approximation is closely related to the two-particle BBGKY set of diagrams; however, there are two important differences. The first essential difference is that because the two VP's are moving independently, there is no constraint dictating that the two VP's cannot move along the same lattice vector at some time step τ. Thus diagrams such as Fig. 20 must be included in this approximation. The second essential difference is that even when the two VP's enter a vertex from different directions described by the state $\hat{i}$ and leave in different directions $\hat{j}$, the amplitude for such a transition is no longer given by $\mathcal{V}$ but rather by the collision matrix U with elements

$$U^{\hat{j}}{}_{\hat{i}} = \delta^j{}_i[(1-2g)(1-3g)] + g(1-g) \ .$$

Despite these differences, it is still possible to formulate an expression for the ring approximation that is identical in form to Eq. (109), where the matrix $\overline{M}$ is no longer defined by Eq. (108) but rather by

$$\overline{M} = M(1-\mathcal{U}M)^{-1} \ ,$$

where the matrix $\mathcal{U}$ has elements $\mathcal{U}^{\hat{j}}{}_{\hat{i}}$ giving the total amplitude for all processes where a pair of particles $\hat{i}$ come together at some vertex, perhaps travel together for several steps, and then separate in directions $\hat{j}$ at the same or a later vertex. Algebraically, $\mathcal{U}$ is given by

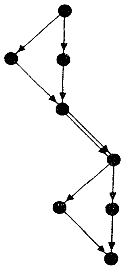


FIG. 20. Unphysical diagram present in the ring approximation.

$$\mathcal{U}=U+ST \ ,$$

where the matrix $T^{k}{}_{\hat{i}}$ gives the amplitude for an incoming pair of particles $\hat{i}$ to both move in direction k according to the separate $\mathcal{V}$ 1-1 vertices and the matrix $S^{\hat{j}}{}_{k}$ gives the total amplitude for a pair of particles both moving in direction k to eventually separate in directions $\hat{j}$. The matrix T can easily be computed from $\mathcal{V}$ and has matrix elements

$$T^{k}{}_{\hat{i}}=\delta^{k}{}_{i}[g(3g-1)]+g(1-2g) \ .$$

The matrix S is slightly more complicated. By symmetry, the elements of this matrix are given by

$$S^{\hat{j}}{}_{k}=\delta^{j}{}_{k}[s-d]+d$$

for some values of the functions $s(g),d(g)$. From the definitions of these functions, one finds that they must satisfy the recursion relations

$$s=2g^2+(1-2g)^2s+2g^2d \ ,$$
$$d=2g(1-2g)+(1-2g)^2d+g^2s+g^2d \ .$$

These equations have the solution

$$s=\frac{-3g}{3g-4}, \quad d=\frac{3g-2}{3g-4} \ .$$

Plugging these values for s and d into S and computing the eigenvalue w of q^2 with respect to the resulting matrix $\mathcal{U}$, we find

$$\mathcal{U}^{\hat{j}}{}_{\hat{i}}=\delta^{j}{}_{i}\left[1-9g\left[\frac{3g-2}{3g-4}\right]\right]+3g\left[\frac{3g-2}{3g-4}\right]$$

and thus

$$w=1-9g\frac{3g-2}{3g-4} \ . \tag{115}$$

As a result of this analysis, we have an expression similar to Eq. (110) for the eigenvalue shift

$$\delta\lambda=9\frac{p^2f(1-f)l}{1-lw} \ , \tag{116}$$

where w is given by Eq. (115). We thus have not only managed to prove that the ring approximation for the 1D3P lattice gas is convergent, but we can also derive from Eqs. (110) and (116) an explicit algebraic relationship between the eigenvalue renormalization from the ring approximation and that from the two-particle BBGKY approximation. If we write the shift in λ due to the ring approximation as δ and the shift from the two-particle BBGKY approximation as δ', we have the equation

$$\frac{\delta(4-3pf)}{\delta(4-21pf+27p^2f^2)+9p^2f(1-f)(4-3pf)} =\frac{\delta'}{\delta'(1-3p+3pf)+9p^2f(1-f)} \ . \tag{117}$$

As a specific example, we can plug in the explicit value of $\delta'\approx-0.012\,550$ for $(p,f)=(0.25,0.5)$, to find that

$$\delta\approx-0.012\,696 \ .$$

This result is in excellent correspondence with numerical calculations.

To derive the correction due to the ring approximation from first principles, note that the weight of any ring diagram is the product of contributions from each of the two virtual particles. Denote by $y^{i}{}_{k}(\mathbf{x},t)$ the factor contributed by a virtual particle beginning at the origin at $\tau=0$ in direction k and terminating at $\mathbf{x}$ at $\tau=t$ in direction i. In terms of these factors, the ring approximation can be written

$$Y^{\{i,j\}}{}_{\{k,l\}}=\sum_{\mathbf{x}}\sum_{t=2}^{\infty}[y^{i}{}_{k}(\mathbf{x},t)y^{j}{}_{l}(\mathbf{x},t) +y^{i}{}_{l}(\mathbf{x},t)y^{j}{}_{k}(\mathbf{x},t)] \ . \tag{118}$$

Because the ring approximation includes only one-point to one-point vertices, the $y^{i}{}_{k}(\mathbf{x},t)$ factors obey the linear, homogeneous dynamical equation

$$y^{i}{}_{k}(\mathbf{x}+\mathbf{c}^{i},t+\Delta t)=\mathcal{V}^{i}{}_{j}y^{j}{}_{k}(\mathbf{x},t) \ .$$

Because this equation is linear and homogeneous, it can be solved exactly in Fourier space. The result can be expressed as a Fourier series in $\mathbf{x}$ and t. When these results for $y^{i}{}_{a}(\mathbf{x},t)$ and $y^{j}{}_{b}(\mathbf{x},t)$, with Fourier summation variables $\mathbf{k}$ and $\mathbf{k}'$, respectively, are inserted into Eq. (118), the summation over time is nothing more than a geometric series and one of the Fourier summations yields a Kronecker δ in $\mathbf{k}$ and $\mathbf{k}'$. The result for $Y^{\{i,j\}}{}_{\{a,b\}}$ is then reduced to one summation over $\mathbf{k}$. Passing to the hydrodynamic limit, this becomes a quadrature. For a D-dimensional lattice gas, one obtains at most a D-dimensional quadrature.

Note that this program can be carried out to compute the ring approximation for any lattice gas. Since the relationship (117) between the ring approximation and the $k=2$ BBGKY truncation is also generalizable to any lattice gas, it follows that the latter approximation is also reduced to quadrature.

E. Comparison of approximations

We conclude this section with a brief discussion of the relative effectiveness of the various methods used to compute partial diagrammatic sums. We have calculated explicitly in this section the corrections to the diffusivity in

TABLE I. Comparison of approximation methods for 1D3P—deviation from Boltzmann theory.

Approximation	$\delta\lambda$		
	$(p,f)=(\frac{1}{4},\frac{1}{2})$	$(p,f)=(\frac{1}{3},\frac{1}{3})$	$(p,f)=(\frac{1}{2},\frac{9}{10})$
Experiment	-0.081 ± 0.0045	-0.0111 ± 0.0022	0.0384 ± 0.0099
$k=5$	-0.0094	-0.0100	0.0414
$k=4$	-0.0095	-0.0106	0.0417
$k=3$	-0.0101	-0.0134	0.0402
$k=2$	-0.0125	-0.0207	0.0441
$\tau=5$	-0.0079	-0.0086	0.0380
$\tau=4$	-0.0046	-0.0006	0.0305
$\tau=3$	-0.0110	-0.0164	0.0319
Ring	-0.0127	-0.0216	0.0373
Boltzmann	0	0	0

the 1D3P lattice gas that arise from various methods of truncating the complete diagrammatic summation. The short-τ approximations seem to converge but require exponential time to compute so that achieving a high degree of accuracy with this method is difficult. The k-particle BBGKY approximations can be calculated in polynomial time and seem to converge rapidly for each value of k. It seems likely that for most other lattice gases of interest, these approximations will behave similarly and thus that in general the BBGKY approximations will be the more efficient of these two methods to achieve a maximal degree of accuracy with a minimum of computation.

We have also discussed the ring approximation and shown that the result of this approximation is closely related to the two-particle BBGKY approximation through an algebraic relation. Since the ring approximation can be performed analytically for most lattice gases, at least in an asymptotic sense, this approximation is generally useful for indicating the convergence properties of the diagrammatic summation for any given lattice gas. In general, for lattice gases in two dimensions that preserve momentum as well as particle number, the ring approximation diverges logarithmically in the lattice size [37]. This divergence can be reproduced from the diagrammatic formalism directly; this issue will be discussed in more detail in a future paper [38].

For the 1D3P lattice gas we have studied in this section, we found that in the vicinity of the parameter value $f=1$, it is possible to expand the sum over diagrams in a power series in $1-f$, giving a perturbation series analogous to the loop expansion in field theory or continuum kinetic theory. We showed that each term in this expansion corresponds to a convergent sum. In other lattice gases, similar expansions may be useful in calculating the effect of renormalization in the vicinity of certain parameter values. When expansions of this type are possible, they are generally more accurate than any of the other approximation methods. Finally, in Table I, we compare numerically the results of the different approximation methods described above to the Boltzmann and computer experimental calculations of the transport coefficients.

IX. CONCLUSIONS

In this paper, we have presented a complete kinetic theory of lattice gases, applied it to four model lattice gases, and compared the predictions of the theory to computer experiment for one of these models. The approach presented in this paper opens up a wide range of possible work on discrete kinetic theory. By applying these techniques to compute deviations from the Boltzmann predictions for commonly used lattice gases, the results of simulations can be more accurately interpreted. Lattice gases are currently being used, both in industrial and academic settings, for computational fluid dynamics calculations; to ensure the accuracy of these calculations, it is essential to account for the renormalization effects that we have studied here.

In addition to quantitative refinement of lattice-gas calculations, the theory presented here provides a tool with which to investigate fundamental physical phenomena in nonequilibrium statistical systems. In recent years, for example, lattice gases have been used to model many different hydrodynamic systems, including reaction-diffusion equations and other systems capable of spontaneous self-organization. It is known [9] that the Boltzmann approximation does not yield accurate results for the transport coefficients of such systems, unless the reactants are allowed to diffuse for several steps between reactions in order to artificially suppress the correlations that develop [39]. These systems strongly violate semidetailed balance, so the methods described in this paper are not directly applicable; nevertheless, in a recent paper [40], we have shown how to extend these methods to accurately describe the non-Gibbsian equilibrium of a lattice gas for the Schlögl model chemical reaction. More generally, these methods will also provide insight into the extremely subtle flow and agglomeration of interparticle correlations, entropy, and information [41] in pattern-forming lattice gases and hence into the dynamical basis of self-organization.

ACKNOWLEDGMENTS

One of us (B.M.B.) would like to acknowledge helpful conversations with and encouragement from Professor

M. H. Ernst, Professor E. G. D. Cohen, and Dr. B. Hasslacher. In addition, he would like to acknowledge the hospitality of the Information Mechanics Group at the MIT Laboratory for Computer Science during a portion of this work. This work was supported in part by the divisions of Applied Mathematics of the U.S. Department of Energy under Contracts Nos. DE-FG02-88ER25065 and DE-FG02-88ER25066.

---

[1] U. Frisch, B. Hasslacher, and Y. Pomeau, Phys. Rev. Lett. **56**, 1505 (1986).

[2] U. Frisch, D. d'Humières, B. Hasslacher, P. Lallemand, Y. Pomeau, and J.-P. Rivet, Complex Syst. **1**, 75 (1987).

[3] H. Chen and W. H. Matthaeus, Phys. Rev. Lett. **58**, 1845 (1987).

[4] D. H. Rothman and J. M. Keller, J. Stat. Phys. **52**, 1119 (1988).

[5] J. A. Somers and P. C. Rem, Physica D **47**, 39 (1991).

[6] C. Burgess and S. Zaleski, Complex Syst. **1**, 31 (1987).

[7] C. Appert, D. H. Rothman, and S. Zaleski, Physica D **47**, 85 (1991); H. Chen, G. D. Doolen, Y. C. Lee, and H. Rose, Phys. Rev. A **40**, 2850 (1989).

[8] B. M. Boghosian and C. D. Levermore, Complex Syst. **1**, 17 (1987).

[9] A. Lawniczak, D. Dab, R. Kapral, and J.-P. Boon, Physica D **47**, 132 (1991).

[10] *Lattice Gas Methods for Partial Differential Equations,* Proceedings of the Workshop on Large Nonlinear Systems, Los Alamos, 1987, Proceedings Volume IV of the Santa Fe Institute Studies in the Sciences of Complexity, edited by G. D. Doolen (Addison-Wesley, Reading, MA, 1990).

[11] *Lattice Gas Methods for PDE's, Theory, Applications and Hardware,* Proceedings of the NATO Advanced Research Workshop, Los Alamos National Laboratory, 1989, edited by G. D. Doolen (North-Holland, Amsterdam, 1991).

[12] *Discrete Kinetic Theory, Lattice Gas Dynamics and Foundations of Hydrodynamics,* Proceedings of the Workshop, Torino, 1988, edited by R. Monaco (World Scientific, Singapore, 1989).

[13] *Cellular Automata and Modeling of Complex Physical Systems,* Proceedings of the Les Houches Winter School of Theoretical Physics, Les Houches, 1989, edited by P. Manneville, N. Boccara, G. Vichniac, and R. Bidaux (Springer, New York, 1989).

[14] *Discrete Models of Fluid Dynamics,* Proceedings of the Colloquium Euromech No. 267, Figueira da Foz, Portugal, 1990, edited by A. S. Alves (World Scientific, Singapore, 1991).

[15] Proceedings of the NATO Advanced Research Workshop, Lattice Gas Automata: Theory, Implementation and Simulation, l'Observatoire de la Côte d'Azur, Nice, 1991, edited by J.-P. Boon and J. L. Lebowitz [J. Stat. Phys. **68**, 347 (1992)].

[16] K. Wilson, Phys. Rev. **179**, 1499 (1969).

[17] L. Boltzmann, Nature **51**, 413 (1895); S. Chapman, Philos. Trans. R. Soc. London Ser. A **216**, 279 (1916); D. Enskog, Svensk. Akad. Handl. **63**, No. 4 (1922).

[18] E. G. D. Cohen, Phys. Today **37**, (1) 64 (1984).

[19] J. R. Dorfman and H. van Beijeren, in *Statistical Mechanics, Part B: Time-Dependent Processes,* edited by B. J. Berne (Plenum, New York, 1977), p. 65, and references contained therein.

[20] See, e.g., E. H. Hauge, in *Transport Processes,* edited by G. Kirczenow and J. Marro, Lecture Notes in Physics Vol. 31 (Springer-Verlag, Berlin, 1974), p. 338.

[21] S. Wolfram, J. Stat. Phys. **45**, 471 (1986).

[22] M. Hénon, Complex Syst. **1**, 763 (1987).

[23] T. R. Kirkpatrick and M. H. Ernst, Phys. Rev. A **44**, 8051 (1991).

[24] See H. J. Bussemaker and M. H. Ernst, in Lattice Gas Automata: Theory, Implementation and Simulation (Ref. [15]), pp. 431–435.

[25] G. A. van Velzen and M. H. Ernst, J. Phys. A **22**, 4611 (1989); G. A. van Velzen, *ibid.* **23**, 4953 (1990).

[26] J. L. Lebowitz, E. Orlandi, and E. Presutti, Physica D **33**, 165 (1988).

[27] Z. Cheng, J. L. Lebowitz, and E. R. Speer, Commun. Pure Appl. Math. **44**, 971 (1991).

[28] R. Brito and M. H. Ernst, J. Phys. A **24**, 3331 (1991).

[29] R. Brito, M. H. Ernst, and T. R. Kirkpatrick, J. Stat. Phys. **62**, 283 (1991).

[30] B. M. Boghosian and C. D. Levermore, in *Proceedings of the Workshop on Discrete Kinetic Theory, Lattice Gas Dynamics and Foundations of Hydrodynamics* (Ref. [12]), pp. 44–61.

[31] R. van Roij, thesis, M. H. Ernst, Institute for Theoretical Physics, University of Utrecht, 1992 (unpublished).

[32] L. Landau and E. Lifshitz, *Fluid Dynamics* (Pergamon, New York, 1959).

[33] J. Zinn-Justin, *Quantum Field Theory and Critical Phenomena* (Clarendon, Oxford, 1989).

[34] C. Itzykson and J. Zuber, *Quantum Field Theory* (McGraw-Hill, New York, 1980).

[35] A. Fetter and J. Walecka, *Quantum Theory of Many-Particle Systems* (McGraw-Hill, New York, 1971).

[36] B. M. Boghosian and W. Taylor (unpublished).

[37] L. Kadanoff, G. McNamara, and G. Zanetti, Phys. Rev. A **40**, 4527 (1989).

[38] B. M. Boghosian and W. Taylor (unpublished).

[39] D. Dab, Ph.D. thesis, Université Libre de Bruxelles, 1992 (unpublished).

[40] B. M. Boghosian and W. Taylor, J. Stat. Phys. (to be published).

[41] T. Toffoli, IBM J. Res. Dev. **32**, 29 (1988).