Renormalization of Lattice Gas Transport Coefficients*

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((November 20, 2018))

A method is described for calculating corrections to the Boltzmann/Chapman-Enskog analysis of lattice gases due to the buildup of correlations. It is shown that renormalized transport coefficients 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 Feynman diagrams of quantum field theory. This theory is applied to an example lattice gas and shown to correctly predict experimental deviation from the Boltzmann prediction.

I. INTRODUCTION

The central problem in the theoretical analysis of a lattice gas is the determination of the macroscopic hydrodynamic equations obeyed by the conserved quantities of the system, with transport coefficients expressed as functions of those conserved quantities. Most analyses of this problem make use of the Boltzmann molecular chaos assumption. This assumption, which neglects correlations between colliding particles, makes possible the derivation of a Boltzmann equation for the single-particle distribution function. For lattice gases satisfying semi-detailed balance, this Boltzmann equation has Fermi-Dirac equilibria. The Chapman-Enskog procedure of linearizing about these equilibria then yields the hydrodynamic equations satisfied by the system. The transport coefficients that appear in these equations are related to the eigenvalues of the linearized Boltzmann collision operator at equilibrium, and these are calculable as functions of the conserved quantities.

Unfortunately, the first step in this analysis – the Boltzmann molecular chaos assumption – is often invalid, and its use can lead to serious errors in the transport coefficients, as has been shown empirically. To see why, recall that the transport coefficients measure the rate at which the propagation/collision process smoothes gradients. These same collisions, however, generate correlations among the bits of the lattice gas, and these correlations can propagate about and subsequently correct the Boltzmann collision operator. Thus, in an exact theory, the renormalized linearized collision operator is the sum of a bare Boltzmann collision operator, and a series of corrections due to the presence of correlations.

*This work was supported in part by Thinking Machines Corporation, in part by the divisions of Applied Mathematics of the U.S. Department of Energy (DOE) under contracts DE-FG02-88ER25065 and DE-FG02-88ER25066, and in part by the U.S. Department of Energy (DOE) under cooperative agreement DE-FC02-94ER40818.
For example, consider 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. This process 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.

In this work, we outline a systematic approach to the exact analysis of a general lattice gas. We show how to construct a diagrammatic series for the transport coefficients of any lattice gas satisfying semi-detailed balance\textsuperscript{1} and we provide closed-form expressions for the vertex coefficients. These results constitute the central part of this paper and are contained in Section 3. The methods that we use here are analogous to the cluster expansion techniques that have been used for many years in the analysis of continuum fluids\textsuperscript{2}. The discrete nature of lattice gases, however, necessitates a construction which differs substantially from the continuum analysis.

The formalism described here is exact, in that it yields the transport coefficients with no approximation. Of course, it is usually a very difficult combinatorial task to sum the diagrammatic series involved, and, more often than not, one must content oneself with an approximation to this series. In doing so, however, it is possible to make contact with other methods of computing this correction. In particular, it is possible to understand kinetic ring theory, and BBGKY truncations in terms of truncations of the exact diagrammatic series, and to characterize the classes of diagrams that they retain, and those that they ignore.

Our analysis differs from previous lattice gas analyses in a few important ways. We formulate the theory in terms of connected correlation functions. A similar expansion in terms of products of fluctuations was previously used in\textsuperscript{3,4} and in\textsuperscript{5,6}, where the ring kinetic theory was derived for lattice gases, and for lattice Lorentz gases, respectively. The use of the connected correlation functions simplifies the form of the complete diagrammatic expansion for the kinetic theory significantly. 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 just to get the Boltzmann approximation.

We describe in Section 4 a variety of simplifications and approximations which 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 2 particles are neglected, and correlations are not allowed to interact. Thus, the results of\textsuperscript{3} are described in our theory by the restriction of the diagrammatic sum to the simple set of ring diagrams.

Finally, to make all this more concrete, in Section 5 a worked example is given, and the results are compared with experiment.

II. 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 $n^i(x, t)$, where $x \in L$ and $i \in B$. These bits can be thought of as a set of occupation numbers for individual particle states. Each of the bits $n^i$ is associated with a lattice vector $c^i$, which represents the velocity vector of the associated particle.

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

\textsuperscript{1}at lowest order
\[ S = \{ s : s \subseteq B \}, \]

where a state \( s \) is associated with the set of bits taking the value 1. 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 1-1 correspondence between the sets \( B = \{1, 2, \ldots, N\} \) and \( B \times L = \{(i, \mathbf{x}) : i \in B, \mathbf{x} \in L\} \). In this notation, a single bit of the lattice gas is written as \( n^a \), \( a \in B \). To relate this notation to the more explicit \((i, \mathbf{x})\) notation, we express the above 1-1 correspondence by writing \( a \) and \((i, \mathbf{x})\) as functions of one another, so that

\[
\begin{align*}
n^a(t) &= n^{i(a)}(\mathbf{x}(a), t) \\
n^i(\mathbf{x}, t) &= n^{a(i, \mathbf{x})}(t).
\end{align*}
\]

We shall use both notations interchangeably throughout this paper.

### III. THE RENORMALIZED CHAPMAN-ENSKOG ANALYSIS

#### A. Ensemble averages

We will denote the mean of an arbitrary product of the \( n^a \)'s by

\[
N^\alpha = \left\langle \prod_{a \in \alpha} n^a \right\rangle, \quad \alpha \subseteq \{1, \ldots, N\}.
\]

There are \( 2^N - 1 \) independent \( N^\alpha \)'s, since \( N^\emptyset = \langle 1 \rangle = 1 \). We will sometimes use a roman index to denote an index set with a single element, as in \( N^a = N^{\{a\}} \).

We introduce an advection operator, \( A_{\alpha \beta}^a \), which is a permutation matrix on the \( 2^N - 1 \) dimensional space of means. \( A_{\alpha \beta}^a \) takes a set of particles \( \beta = \{b_1, \ldots, b_q\} \) to the advected set of particles \( \alpha = \{a_1, \ldots, a_q\} \), where \( a_j = a(i(b_j), \mathbf{x}(b_j) + c(b_j)) \). Note that this generalizes the usual concept of an advection operator, that propagates single particles from site to site, to one that can propagate arbitrary multipoint quantities (e.g., connected correlation functions) from site to site.

#### B. Boltzmann Analysis

The evolution of a lattice gas in one time step can be divided into two parts. The first part is a collision phase in which the \( n \) bits at each point alter their values in some specified way. The second part is a propagation phase in which the value of each bit moves to the corresponding bit of the lattice point to which it is carried by its associated velocity vector. The complete time-development equation is then written as

\[
n^i(\mathbf{x} + \mathbf{c}^i, t + \Delta t) = n^i(\mathbf{x}, t) + \omega^i \left( n^*(\mathbf{x}, t) \right).
\]

The collision operator \( \omega^i \) is generally a nonlinear function of its arguments. Note that the form \( f(\mathbf{z}^*) \) is used to indicate that a function \( f \) depends on a quantity \( \mathbf{z} \) for all possible values of the index \( * \).

The Boltzmann molecular chaos assumption can be written

\[
\left\langle \omega^i \left( n^*(\mathbf{x}, t) \right) \right\rangle \approx \omega^i \left( \left\langle n^*(\mathbf{x}, t) \right\rangle \right).
\]

This is inexact when \( \omega^i \) is nonlinear.

Taking the ensemble average of Eq. (III.1), and making the molecular chaos assumption leads to the Boltzmann equation,
\[ N^b(t + \Delta t) = A_c^b \left( N^c(t) + \Omega^{(c)} \left( N^{a(s, x(c))}(t) \right) \right), \]  

(III.2)

where repeated indices (c in this case) are summed. This is a closed system of equations for the \( N^a \)'s.

The usual Chapman-Enskog analysis proceeds by expanding this equation of motion using Navier-Stokes ordering: A formal expansion parameter \( \epsilon \) is introduced, such that \(|c|^\epsilon \sim \epsilon \). The time step is ordered as \( \Delta t \sim \epsilon^2 \), as is appropriate for viscous or diffusive processes. Since the lattice gas is assumed to satisfy semi-detailed balance, there is a Fermi-Dirac equilibrium. It is assumed that deviations from this equilibrium are of order \( \epsilon \). We will denote the equilibrium values of the single-particle means by \( N^\text{eq}_a \).

Expanding the collision operator in (III.2) to first order in \( \epsilon \) gives

\[ N^b(t + \Delta t) = A_c^b \left( N^c(t) + \epsilon J^{ij(c)} N^{a(i, x(c))}(t) \right). \]  

(III.3)

where \( J^{ij} = \partial \Omega^i(N^*)/\partial N^j \) is the Jacobian matrix of the collision operator evaluated at the equilibrium.

The rest of the Chapman-Enskog analysis consists of associating the hydrodynamic and kinetic modes of the system with eigenvectors of \( J \), and writing the hydrodynamic equations in such a way that the transport coefficients are functions of the eigenvalues of \( J \). For a more in-depth review of the details of this procedure, see.

C. Exact Analysis

We will now drop the Boltzmann assumption and show that the exact equation of motion leads in the scaling limit to an equation identical to (III.3), but with a renormalized \( J \) matrix. We will expand about the same equilibrium as in the usual analysis. For any lattice gas satisfying semi-detailed balance, this equilibrium exists; in the vicinity of this equilibrium, correlations of at most order \( \epsilon \) are generated in a single time step.

We begin with the exact time-development equation (III.1). By taking the ensemble average of the product of this equation over all \( a \) in an arbitrary set \( \alpha \subseteq B \), 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

\[ N^\alpha(t + \Delta t) = \left( \prod_{a \in \alpha} n^a(t + \Delta t) \right) = \sum_{\beta} A^\alpha_{\beta} \left( \prod_{b \in \beta} \left[ n^b(t) + \omega^{i(b)}(n^s(x(b), t)) \right] \right). \]  

(III.4)

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 \( \beta \subseteq B \), let us define \( L_\beta \) to be the subset of points in \( L \) which contain at least one particle in the set \( \beta \); that is, \( L_\beta = \{ y \in L : x(b) = y \text{ for some } b \in \beta \} \).

Similarly, we define \( \beta_x \) to be the set of \( i \)'s corresponding to the particles in \( \beta \) at the point \( x \); that is, \( \beta_x = \{ i \in B : a(i, x) \in \beta \} \).

We can now factorize the product appearing on the right-hand side of (III.4) into contributions from each of the points in \( L_\beta \), by writing

\[ \prod_{b \in \beta} \left[ n^b(t) + \omega^{i(b)}(n^s(x(b), t)) \right] = \prod_{x \in L_\beta} \prod_{i \in \beta_x} \left[ n^i(x, t) + \omega^{i}(n^s(x, t)) \right]. \]

The innermost product on the right now depends only on quantities at a single site, \( x \).

The functions \( \omega^i(n^s) \) can be expressed as polynomials in the \( n^j \)'s of the form \( \omega^i(n^s) = \sum_{\nu \subseteq B} h^i_{\nu} \prod_{j \in \nu} n^j \).
where the \(k_i^\nu\) are coefficients which may depend only on stochastic variables at each lattice site, and which are constant for deterministic lattice gases. Thus, we can write
\[
\prod_{i \in \mu} [n_i + \omega_i(n^*)] = \sum_{\nu \subseteq B} v^\mu_\nu \prod_{j \in \nu} n^j,
\]
where the quantities \(v^\mu_\nu\) may contain stochastic variables at each site. Taking the ensemble average over any such variables, we get the mean vertex coefficients \(V^\mu_\nu\).

The lattice gas state transition probabilities \(A(s \rightarrow s')\) may be interpreted as elements of a collision matrix on the space of probabilities, \(P^s\), in the sense that the post-collision probability of a state \(s'\) is given by
\[
\sum_s A(s \rightarrow s') P^s.
\]
Similarly, the matrix \(V^\mu_\nu\) can be interpreted as a collision matrix on the space of means. Since the probabilities and the multipoint means are straightforwardly related, it is possible to relate the matrix \(V\) to the transition probabilities. We get
\[
V^\mu_\nu = \sum_{s' \supseteq \mu} \sum_s (-1)^{|\nu| - |\mu|} A(s \rightarrow s'),
\]
where we have identified the state \(s\) with the set of bits which are 1 in that state \((s \subseteq B)\). Clearly, the \(2^{2n}\) matrix elements \(V^\mu_\nu\) depend only on the sets \(\mu\) and \(\nu\), and on the form of the collision operator. In particular, they do not depend on \(x\), or on the values of the \(n^\alpha\)'s. Note that \(V^\emptyset_\nu = \delta^\emptyset_\nu\), regardless of the specific lattice gas or collision rule.

Eq. (III.4) can now be rewritten in the form
\[
N^\alpha(t + \Delta t) = A^\alpha_\beta K^\gamma K^\mu N^\gamma(t),
\]
where \(K\) is an operator expressing the complete collision part of the time development, given by
\[
K^\beta_\gamma = \prod_{x \in L_a} V^\beta_x^\gamma_x.
\]

We shall now rewrite the dynamical equation (III.8) in the language of connected correlation functions (CCF's). For each \(\alpha \subseteq \{1, \ldots, N\}\), there is a CCF, written \(\Gamma^\alpha\). It is simplest to relate the CCF's to the means by the equation
\[
N^\alpha = f^\alpha(\Gamma^*) = \sum_{\pi(\alpha)} \Gamma^{\zeta_1} \cdots \Gamma^{\zeta_q},
\]
where \(\pi(\alpha)\) is the set of all partitions of \(\alpha\) into disjoint subsets, \(\zeta_1, \ldots, \zeta_q\). Thus, for example, we have \(N^\alpha = \Gamma^\alpha\) and
\[
N^{abc} = \Gamma^{abc} + \Gamma^a \Gamma^{bc} + \Gamma^b \Gamma^{ac} + \Gamma^c \Gamma^{ab} + \Gamma^a \Gamma^b \Gamma^c.
\]
For notational convenience, an index set with a circumflex, e.g. \(\hat{\alpha}\), is assumed to have at least two elements. We refer to the mean (CCF) of a set with \(q\) elements as a \(q\)-mean (\(q\)-CCF).

Equation (III.10) can be inverted by induction on \(|\alpha|\) to get an expression of the form \(\Gamma^\alpha = g^\alpha(N^*)\), where \(g = f^{-1}\). We can now use \(f\) and \(g\) to convert (III.8) into a dynamical equation for the CCF's, giving
\[
\Gamma^\alpha(t + \Delta t) = A^\alpha_\beta \Phi^\beta(\Gamma^*),
\]

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Similarly, when we include the effects of correlations to order $\epsilon$

\[ \Phi^\beta(\Gamma^*) \equiv g^\beta(K^* g^\gamma(\Gamma^*)) ; \]

we have used the fact that $A$ is a permutation matrix, so that $g$ and $A$ commute.

For an ensemble of independent variables, all CCF’s except the 1-CCF’s vanish. The equilibrium distribution is such an ensemble, so we can take any term $\Gamma^\alpha$ to be of order $\epsilon$. In the asymptotic analysis, only first order terms in $\epsilon$ need be kept in the expression $\Phi^\beta(\Gamma^*)$. Thus, the dynamical equation for the CCF’s can be linearized to

\[ \Gamma^\alpha(t + \Delta t) = A^\alpha_{\beta} \left( \epsilon K^\beta_{\gamma} N^\alpha_1(t) + K^\beta_{\gamma} \Gamma^\gamma(t) \right), \]

(III.12)

where

\[ K^\beta_{\gamma} = \frac{\partial \Phi^\beta}{\partial \Gamma^\gamma} \bigg|_0 = \frac{\partial g^\beta}{\partial N^\gamma} \bigg|_0 K^\sigma \frac{\partial f^\tau}{\partial \Gamma^\gamma} \bigg|_0. \]

(III.13)

Similarly, when we include the effects of correlations to order $\epsilon$ in (III.11) for $\alpha = \{a\}$, the dynamical equation for $N^a = \Gamma^a$ becomes

\[ N^a(t + \Delta t) = A^a_b \left( N^b(t) + \epsilon [K^b_{\gamma} \delta^b_{\gamma} - \delta^b_{\gamma}] N^c_1(t) + K^b_{\gamma} \Gamma^\gamma(t) \right). \]

(III.14)

Note that if we set $\hat{\Gamma}^\alpha = 0$ in this equation, we get back the linearized Boltmann equation (III.3), since

\[ K^b_{\gamma} \delta^b_{\gamma} = \delta^x(b) x(c) J^{i(b)}_{i(c)}. \]

Inserting (III.12), we can now write the exact equation of motion for the quantities $N^a$ in the form of an infinite series,

\[ N^a(t + \Delta t) = A^a_b \left( N^b(t) + \epsilon J^b_{c} N^c(t) \right), \]

(III.15)

where

\[ J^b_{c} = \delta^x(b) x(c) J^{i(b)}_{i(c)} + K^b_{\alpha} (A^\alpha_{\beta} K^\beta_{\gamma}) + A^\alpha_{\beta} K^\beta_{\gamma} (A^\gamma_{\delta} K^\delta_{\epsilon} + \ldots)). \]

(III.16)

We now have an expression for the mean occupation number of a certain bit of the system at position $x$ 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 $x'$ and at previous time steps $t'$. As we consider terms in this series with more and more factors of $AK$, the positions and times at which these quantities are evaluated will differ from $x$ and $t$ by greater amounts. However, for any given term in the series, the means $N^a_0(i,x')(t')$ and $N^a_1(i,x')(t')$ can be replaced by $N^a_0(i,x)(t)$ and $N^a_1(i,x)(t)$, and the expression (III.16) will only change by a quantity of order $\epsilon$, since spatial derivatives are ordered as $\epsilon$, and temporal derivatives are ordered as $\epsilon^2$. 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 (III.16) converges on a scale which goes to zero in the hydrodynamic limit, we can drop all the spatial and temporal variations in the single-particle means. Thus, (III.15) can be rewritten in precisely the form of Eq. (III.3), where $J$ is replaced by the renormalized matrix

\[ \tilde{J}^i_{j}(x) = \sum_{y \in L} J^{a(i,x)}_{a(j,y)}, \]

(III.17)

with all $K$’s in $J$ evaluated at the point $x$ and the time $t$. 

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It is important to note that the above argument breaks down when the sum (III.16) is divergent. In this case, the effects of large scale variations in the \( N^a(i,k) \)'s must be considered. In general, for lattice gases where (III.16) is divergent, one must be quite careful about the analysis. For certain lattice gases, however, particularly systems in which the conserved quantities are ordered, we are interested in expanding around an equilibrium which is spatially invariant (for example, the FHP-I lattice gas). In this case, the zero-order means can be replaced by their universal values; however, one must still treat the spatial variation of the first-order means carefully.

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 \( \tilde{J}_j \) in the same way that the original (Boltzmann) transport coefficients were related to the eigenvalues of the matrix \( J_j \). Thus, if we can compute the matrix \( \tilde{J}_j \) exactly, we can also compute the exact renormalized transport coefficients.

We will now show that expression (III.16) 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 key observation which allows this reduction is the following:

**Theorem 1** For fixed \( \alpha \) and \( \beta \), \( \mathcal{K}^{\alpha \beta} \) can be broken down into a product of contributions from distinct vertices. Explicitly,

\[
\mathcal{K}^{\alpha \beta} = \prod_{x \in L_\alpha} V^{\alpha x}_{\beta_x}, \tag{III.18}
\]

where the correlation vertex coefficients (CVC’s), \( V \), are defined by

\[
V^{\alpha x}_{\beta_x} = \sum_{\mu, \nu} (-1)^{|\alpha_x \setminus \mu| \left( \prod_{i \in (\alpha_x \setminus \mu)} N_0^i \right) \left( \prod_{j \in (\nu^c \setminus \beta_x)} N_0^j \right) V^\mu_\nu}, \tag{III.19}
\]

with the sum taken over \( \mu \subseteq \alpha_x \) and \( \nu \supseteq \beta_x, \nu \subseteq B \).

This theorem can be proven by expressing \( \partial f^a / \partial \Gamma^\beta \bigg|_0 \) and \( \partial g^a / \partial N^\beta \bigg|_0 \) as products of the \( N_0 \) and plugging into (III.13). For a full derivation see \[\text{[Ref]}\]. Using this result, it is possible to express every term in \( \mathcal{J}_h \) in diagrammatic form. A general nonzero term is given by

\[
\mathcal{K}^{\alpha^k \beta^k} A^{\beta^k}_{\alpha^k-1} \mathcal{K}^{\alpha^{k-1} \beta^{k-1}} \cdots A^{\beta^2}_{\alpha^1} \mathcal{K}^{\alpha^1 \beta^1} \tag{III.20}
\]

with \( \alpha^i \) and \( \beta^i \) fixed (i.e., not summed over), and \( |\alpha^i|, |\beta^i| \geq 2 \), except for the endpoints 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 \( \tau \in \{0, \ldots, k\} \), \( \alpha_T(\tau) \subseteq B \). Geometrically, we associate each \( a \in \alpha_T(\tau) \) with a virtual particle (VP) moving from \( (x(a), \tau) \) to \( (x(a) + c^{(a)}, \tau + 1) \) 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 \( \beta_T(\tau) = \{b : a(i(b), x(b) - c^{(b)}) \in \alpha_T(\tau - 1)\} \). We also define \( \sigma_T(\tau) = |\alpha_T(\tau)| \) to be the total number of outgoing VP’s for each value of \( \tau \). Finally, given a diagram \( T \), we can define a weight function

\[
W(T) = \prod_{x \in L} \prod_{1 \leq \tau \leq k(T)} V^{\alpha_T(\tau)_x}_{\beta_T(\tau)_x},
\]

by taking the product of \( V \) over all vertices.

The term (III.20) can now be represented by the diagram \( T \) with \( \alpha_T(\tau) = \alpha^\tau \), where for consistency \( \alpha^0 \) is defined to be the unique set with \( A^\alpha_{\alpha^0} = 1 \). When \( \tau \neq 0 \), \( A^{\beta^{\tau+1}}_{\alpha^\tau} = 1 \), so \( \beta_T(\tau) = \beta^\tau \) for all \( \tau \). It follows
that the contribution from (III.20) is exactly given by $W(T)$. Thus, we can rewrite expression (III.16) for $\mathcal{J}^a_b$ as a sum over diagrams

$$\mathcal{J}^a_b = \sum_{k=1}^{\infty} \sum_{T \in T^a_b(k)} W(T),$$

where in general we define the set of diagrams $T^\alpha_\beta(k)$ by

$$T^\alpha_\beta(k) = \{ T : k = k(T), \sigma_T(l) > 1, \text{ for } 1 \leq l < k, \alpha_T(k) = \alpha, \beta_T(1) = \beta \}.$$

Note that $V^\emptyset_\nu = \delta^\emptyset_\nu$, so any diagram with incoming VP’s at $(x, t)$ but no outgoing VP’s has weight zero. For many lattice gases certain other vertex factors $V^\mu_\nu$ vanish also; diagrams with such vertices can be dropped from the sum (III.21). From (III.17), $\tilde{J}$ can now be written as a sum over diagrams in the same fashion as $\mathcal{J}$,

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

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

$$T^i_j(x, k) = \bigcup_{b:1(b)=j} T_a^{(i, x)}_b(k).$$

IV. 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 which we can make to truncate the series to one which is summable. The questions of convergence are rather difficult, and we will not address them here; 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 have been applied to related problems in quantum field theory and quantum many-body theory\textsuperscript{8,9}. We will describe here several particular approximation methods which are useful for the kind of series which arise for known lattice gases.

A. Short-$\tau$ and Small-$\ell$ Truncations

The simplest useful approximations involve truncating the sum (III.21) to a finite number of terms by putting an upper bound on either the number of timesteps or the number of distinct nontrivial vertices allowed in each diagram. In the first case, the expression for the renormalized $J$-matrix is

$$\tilde{J}_{j}^{(\tau)}(x) = \sum_{k=1}^{\tau} \sum_{T \in T^i_j(x,k)} W(T),$$

where the diagrams summed over are the same as those summed in Eq. (III.22). Since for each fixed value of $k$ there are a finite number of allowed diagrams, this sum is finite. We refer to this approximation as the short $\tau$ approximation. In the second case, we allow $k$ to be arbitrary, but allow only diagrams where the total
number of vertices \((x, k')\) with nonempty outgoing sets \(\alpha_T(k')_x\) is less than or equal to some fixed number \(\ell\). We denote the sum restricted to these diagrams by \(\tilde{J}^{[\ell]}\). Again, there are 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 \(V_{\mu \nu}\) are usually not particularly small. The short-\(\tau\) and small-\(\ell\) truncations give good consecutive approximations for many lattice gases, and in most instances pick out the contributions to the renormalization of the transport coefficients in decreasing order. In either of these two approximations, the Boltzmann approximation can be recovered, by taking \(\tau = 1\) or \(\ell = 1\).

**B. 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 \(\sigma_T(k') \leq n\) for \(1 \leq k' \leq k\). Whereas the total number of distinct diagrams in the complete sum grows exponentially in \(k\), the number of distinct diagrams in the BBGKY approximations grow polynomially, and are computationally more tractable.

**C. The 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 which model two dimensional fluid systems, the ring approximation diverges logarithmically in \(|L|\), which is in agreement with predictions from other theoretical frameworks\(^3\), and also with observed behaviour\(^1\).

**V. THE 1D3P LATTICE GAS**

As a simple example, we consider a diffusive lattice gas model in one dimension. 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 \(\tilde{\phantom{t}} \equiv \{-, 0\}, 0 \equiv \{-, +\}, \) and \(\tilde{\phantom{t}} \equiv \{0, +\}\), then the nontrivial elements of the state transition table can be written

| \(a(s \rightarrow s')\) | \(s'\) | \(\tilde{\phantom{t}}\) |
|----------------------|------|------|
| +                   | 1 - \(n_p\) | \(n_p(1 - n_r)\) |
| 0                   | \(n_p n_r\) | 1 - \(n_p\) |
| \(\tilde{\phantom{t}}\) | \(n_p (1 - n_r)\) | \(n_p n_r\) | \(1 - n_p\) |

The bits \(n_p\) and \(n_r\) are stochastic bits\(^2\) which are sampled separately at each lattice site and at each timestep with average values \(\langle n_p \rangle = 2p\) and \(\langle n_r \rangle = 1/2\). Here, the parameter \(p \in [0, \frac{1}{2}]\) may be thought of as the

\(^2\)Note that \(r\) and \(p\) are not indices here, but rather simply labels for the stochastic bits.
probability of collision from, e.g., $\hat{\mathbf{t}}$ to $\mathbf{0}$. 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 obey semi-detailed balance, since the columns of the above table sum to unity. Also note that they conserve particles ($n_c = 1$); it is the particle density $f$ that will obey the macroscopic diffusion equation.

Beginning with the above state transition table, we can calculate the mean vertex coefficients $V^\mu_\nu$ using equation (III.5) or (III.7). The nonzero mean vertex coefficients are given by

$$V^B_B = V^\emptyset_\emptyset = 1$$

$$V^i_j = \delta^i_j$$

$$V^\bot_j = p(3\delta^i_j - 1)$$

$$V^\bot_j = p + \delta^i_j(1 - 3p).$$

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

The nonvanishing correlation vertex factors are depicted graphically in Figure 1; only a single vertex is shown in each equivalence class under the permutation symmetry. Note that the CVC’s are also symmetric under an arbitrary permutation on the particle labels.

\begin{align*}
V^0_0 &= 1 - 2pf \\
V^-_0 &= pf \\
V^+_0 &= -pf(1 - f) \\
V^-_0 &= 2pf(1 - f) \\
V^0_0 &= -p \\
V^-_+ &= 2p \\
V^+_+ &= p(1 - f) \\
V^-_+ &= 1 - 2p(1 - f) \\
V^B_B &= 1
\end{align*}

FIG. 1. Vertex Factors for 1D3P Lattice Gas
The Chapman-Enskog analysis for this lattice gas is straightforward, and yields the following expression for the diffusivity in terms of the kinetic eigenvalue, $\tilde{\lambda}^2$:

\[
\tilde{D} = \frac{c^2}{3\Delta t} \left( \frac{2}{-\tilde{\lambda}^2} - 1 \right). \tag{V.1}
\]

The Boltzmann value for $\tilde{\lambda}^2$ is $-3pf$. The renormalized result can be written

\[
\tilde{\lambda}^2 = -3pf + 9p^2f(1-f) \left( \sum \ldots \sum \ldots \right), \tag{V.2}
\]

where the notation in brackets indicates summation of the products of all internal vertex factors over all diagrams with the depicted initial and final configurations. Together, Eqs. (V.1) and (V.2), with vertices given in Figure 1, constitute an exact expression for the diffusivity of the 1D3P lattice gas.

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 $\leq \tau$ on a lattice of width $l$, then to take the limits as $\tau, l \to \infty$. In this way, we have numerically approximated the limits of the $k$-particle BBGKY sums for $k < 6$. The results of this calculation, plotted as the correction to the Boltzmann value of the kinetic eigenvalue, versus mean occupation number, are graphed in Figure 2 for $p = 1/2$. It is especially noteworthy that when $f = 1/2$ the ring approximation and lower BBGKY truncations are inadequate (indeed, the $k = 2$ and ring truncations actually get the wrong sign for the correction), but the $k = 5$ BBGKY truncation does quite well indeed.

\[0.05\]
\[0.04\]
\[0.03\]
\[0.02\]
\[0.01\]
\[0\]
\[-0.01\]
\[-0.02\]
\[-0.03\]
\[-0.04\]
\[-0.05\]
\[0\]
\[0.2\]
\[0.4\]
\[0.6\]
\[0.8\]
\[1\]

\[\delta \lambda^2\]

\[f\]

\[k = 2\]
\[k = 3\]
\[k = 4\]
\[k = 5\]

\[\text{experiment}\]

FIG. 2. Partial BBGKY Approximations for $p = 1/2$

VI. CONCLUSIONS

In this paper, we have outlined a complete kinetic theory of lattice gases, applied it to a simple model lattice gas, and compared the predictions of the theory to experiment.
The approach presented in this paper opens up a wide range of possible new 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 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. Thus, it is likely that the methods described in this paper will be directly applicable to these systems, providing an important correction to their theory. More interestingly, these methods will also provide insight into the extremely subtle flow and agglomeration of interparticle correlations in pattern-forming lattice gases, and hence into the dynamical basis of self-organization.

ACKNOWLEDGEMENTS

One of us (BMB) would like to acknowledge helpful conversations with and encouragement from Professors M.H. Ernst and E.G.D. Cohen, and from Dr. B. Hasslacher. In addition, he would like to acknowledge the hospitality of the Information Mechanics Group at the M.I.T. Laboratory for Computer Science where he was a visiting scientist during a portion of this work. This work was supported in part by Thinking Machines Corporation, in part by the divisions of Applied Mathematics of the U.S. Department of Energy (DOE) under contracts DE-FG02-88ER25065 and DE-FG02-88ER25066, and in part by the U.S. Department of Energy (DOE) under cooperative agreement DE-FC02-94ER40818.

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