PROCEEDINGS OF THE INTERNATIONAL SYMPOSIUM
ON LUDWIG BOLTZMANN
(ROME, FEBRUARY 9–11, 1989)

EDITED BY

GIOVANNI BATTIMELLI · MARIA GRAZIA IANNIELLO
OTTO KRESTER

Separata

Wien 1993

VERLAG DER
ÖSTERREICHISCHEN AKADEMIE DER WISSENSCHAFTEN
1. Introduction

My purpose in this lecture is to discuss some of the current applications and extensions of Boltzmann’s ideas in the area of condensed matter science. Since I am not a historian, accuracy is best served by confining my remarks to areas in which I have carried out my own research, namely to a series of topics concerned with the liquid state.

The first topic I will discuss is the so-called “van der Waals picture” of liquids. This simple model for real gases and liquids and the transition between them was a primary interest for the practitioners of statistical mechanics at the end of the 19th century. Boltzmann played an important role in the developing of theories for the analysis of this model (often correcting mathematical oversights by van der Waals himself) [1]. It is remarkable that this model is still of great importance in liquid state science today [2].

A second topic is the extension of the van der Waals model to treat complicated molecular fluids. Here, as in the atomic fluid case, entropic effects – the available configurational space – is of paramount importance. But for molecular fluids, one must account for the constraints of chemical bonding which diminish the space sampled when performing Boltzmann weighted sums over atomic configurations. I have developed a mathematical theory that captures this entropic feature [3], and I will describe representative applications.

The constrained Boltzmann weighted sum over atomic configurations is isomorphic to Feynman’s prescription for performing quantum mechanical calculations, the sum over quantum paths [4]. The last topic of this lecture concerns this mapping. With Feynman’s formulation of quantum mechanics, nearly all of contemporary science is placed into one unified structure, the creation of which begins with Boltzmann’s work.

2. The Van der Waals Picture of Liquids

Consider the interactions between closed shell atoms. They are attractive at large distances, and repulsive at short distances. The attractions are due to correlations between the small amplitude charge fluctuations on the different atoms. These
are London's dispersion interactions. The repulsions are due to a different mechanism, Pauli's exclusion principle. Due to adherence to this principle, the overlap of two closed shell atoms must lead to excitations in atomic electronic states. The energies associated with the electronic excitations are very large compared to Boltzmann's thermal energy, $k_B T$. On the other hand, the most favorable London attractions are never much larger than $k_B T$.

With these ideas in mind, imagine now a simple liquid, a dense fluid composed of noble gas atoms such as liquid argon. Consider the energetics associated with moving one of the atoms. Because the density is high, the most significant contributions to the energetics will be due to the interparticle interactions with the largest magnitude of forces. The repulsive branch, as we have noted above, is by far the largest in this sense. Therefore, the arrangement of atoms in a dense fluid will be determined by the repulsive forces.

Will the attractions do anything? Surely they will provide a mean background potential which makes the dense fluid macroscopically stable. But once the liquid is stable, one might expect that the atoms are arranged and move about as if the repulsions were the only forces.

This idea can be traced back to the time of Boltzmann and van der Waals. These scientists did not know the quantum mechanical mechanism for interatomic forces. Boltzmann did, however, understand the physical model upon which the celebrated van der Waals equation is based -- hard spheres with relatively weak and relatively long ranged interparticle attractions [5]. For such a model, the idea that repulsive forces or packing effects dominate the liquid structure is obviously correct since the attractions are weak and long ranged and therefore exert no appreciable forces. What is truly remarkable is that this van der Waals model or picture of liquid structure is a reasonable caricature of real liquids where the attractions are not so obviously weak. The reason is that packing effects or jamming of particles at high densities in effect quench the density fluctuations for which attractive energies might change appreciably. In other words, the repulsive forces screen the attractions and thereby make the van der Waals model an acceptable model of liquids.

This understanding is the result of contributions of many scientists. Among the most relevant is the discovery with computer modeling by Alder and Wainwright [6] and by Wood and Jacobs [7] that a fluid of hard spheres will freeze when compressed to certain finite pressure, and the demonstration by Longuet-Higgins and Widom [8] that this transition underlies the solidification of real liquids such as argon. Also important was Verlet's use of the hard sphere model to empirically fit the structure factors of liquid argon which he computed by molecular dynamics [9]. Weeks, Andersen and I were able to quantify the connection between the hard sphere model and more realistic models with
Fig. 1: Structure and pair interactions of a simple liquid. A schematic view of a region of a liquid composed of spherical particles interacting via a pair potential \( w(r) \) is shown in the upper right. The dashed circle depicts the displacement referred to in the text, the repulsive branch of the potential, \( u_r(r) \), is indicated by a solid curve. The WCA associated hard sphere potential, \( u_h(r) \), which is infinite for \( r<d \) and zero otherwise, is shown schematically with \( w(r) \). The radial distribution function, \( g(r) \), for the Lennard-Jones liquid at a state near the triple point is plotted and compared with \( g_0(r) \) and \( g_d(r) \), the radial distribution functions of the repulsive force systems with pair potentials \( u_r(r) \) and \( u_h(r) \) at the same temperature and density. (After Chandler [11] and Chandler et al. [2].)
continuous forces with a statistical mechanical analysis that is now usually referred to as WCA (Weeks-Chandler-Andersen) theory [10].

Figure 1, adapted from two reviews [2, 11], illustrates the most important conclusions drawn from this work: the structure of atomic fluids are determined primarily by the short ranged quickly varying repulsions acting between atoms, and the effects of these repulsions are essentially the same as those due to infinitely rapidly varying repulsions - the hard sphere model. Thus, a child playing with a box of marbles can view the essential features of liquid structure, and by packing the box to a high enough density in regular fashion, the child may witness freezing too.

3. Complex Fluids, Reference Interactions Site Model

How might these ideas be used when considering more complicated systems, liquids composed of nonspherical molecules?

The problem can be viewed in this way. Molecules are collections of atoms. Therefore, as in the case of simple fluids, the statistical mechanics for such systems corresponds to Boltzmann weighted sampling of atomic configurations. But unlike the atomic fluid case, the configuration space for a molecular fluid is reduced by the constraints of chemical bonding. In other words, chemical bonding leads to an entropy reduction. For long wavelength fluctuations, the constraints of chemical bonding are the conditions of stoichiometry. On shorter microscopic length scales, the constraints lead to more specific structural features as illustrated for a simple case in Fig. 2. The phenomenological framework used to discuss these effects is a perspective known as the reference interaction site model, or RISM. I will describe this picture now in its simplest form.

Let \( g_{\alpha\gamma}(r) \), denote the pair distribution function between an atom \( \alpha \) located at the origin and an atom \( \gamma \) of another molecule at position \( r \). We adopt the convention where \( g_{\alpha\gamma}(r) \) is unity when these atoms are uncorrelated. So,

\[
\hat{h}_{\alpha\gamma}(r) = g_{\alpha\gamma}(r) - 1
\]

is the pair correlation function for the fluid, and it satisfies the boundary condition \( \hat{h}_{\alpha\gamma}(r) \to 0 \) as \( r \) grows to be much larger than any correlation length. Now, one way in which the two atoms might be correlated is that the pair of molecules they are associated with are so close together that the atoms are actually touching. The contribution to such a configuration we will call \( c_{\alpha\gamma}(r) \), where \( c_{\alpha\gamma}(r) \) is an effective coupling, in units of \(-k_BT\), mediated by the surrounding liquid.
Another contribution might involve a linear sequence perhaps like

$$\sum_{\eta, \lambda, \xi} \int dr' \int dr'' \int dr''' s_{\eta\lambda}(r') c_{\lambda\eta}(|r' - r''|) \rho \ s_{\xi\zeta}(|r'' - r'''|) \ c_{\xi\eta}(|r''' - r|)$$

where the sums are over all the atoms ("interaction sites") in a molecule, $\rho$ is the bulk density and $s_{\eta\lambda}(r)$ is the intramolecular pair distribution. This integral and sum can be represented in a physically suggestive diagrammatic notation as

![Diagram](image-url)
where the wavy lines are $s$-bonds depicting the $s$-function, the straight lines are $c$-bonds. These bonds connect pairs of atoms, the vertices in the diagram. The blackened ones are integrated or summed over all possibilities; they are called field points. The white ones are called roots; they fix particular particles at particular points in space and are thus labeled. Notice that the illustrated diagram involves three different molecules. Two of them are associated with the tagged pair of atoms, $\alpha$ and $\gamma$. The other one, the intermediate molecule in the chain, is any other molecule. The density of such intermediate molecules is $\rho$, so the diagram has one power of $\rho$ associated with its value.

The previous paragraph is a synopsis of some diagrammatic or graph theoretic terminology and notation that is common in all of contemporary statistical mechanics. These diagrams are useful in visualizing physical processes, especially when they refer to paths as discussed in the next section. The diagrams are also useful as a tool for manipulating equations as we will use them now.

Imagine as a mechanism for pair correlations all possible linear sequences, the diagram shown above is only one example. That is,

\[
\begin{align*}
    h_{\alpha \gamma}(r) &= \gamma + \alpha \gamma \gamma + \alpha \gamma \gamma + \alpha \gamma \\
    &\quad + \alpha \gamma \gamma \gamma + \cdots \\
    &\quad + \alpha \gamma \gamma \gamma \gamma \gamma \gamma + \cdots 
\end{align*}
\]

This infinite sequence can be regrouped as

\[
\begin{align*}
    h_{\alpha \gamma}(r) &= \gamma + \alpha \gamma \gamma + h
\end{align*}
\]

where

\[
\begin{align*}
    \gamma &= \alpha + \alpha \gamma
\end{align*}
\]

This infinite sequence can be regrouped as

\[
\begin{align*}
    h_{\alpha \gamma}(r) &= \gamma + \alpha \gamma \gamma + h
\end{align*}
\]

where

\[
\begin{align*}
    \omega_{\alpha \gamma}(r - r') &= \delta_{\alpha \gamma} \delta(r - r') + (1 - \delta_{\alpha \gamma}) s_{\alpha \gamma}(r - r'). 
\end{align*}
\]

Or, in nondiagrammatic notation,

\[
\begin{align*}
    h_{\alpha \gamma}(r) &= \sum_{\eta, \lambda} \omega_{\eta \lambda} c_{\eta \lambda} \left[ \omega_{\lambda \gamma}(r) + \rho h_{\lambda \gamma}(r) \right]
\end{align*}
\]

where the $*$ denotes the convolution integral.
Equation (3.6) is the Chandler-Andersen equation [12]. It expresses the pair correlation functions, $h_{\alpha\gamma}(r)$, in terms of the intramolecular distributions and the direct correlation functions, $c_{\alpha\gamma}(r)$. Long ago, in effect, Ornstein and Zernike also expressed the pair correlation functions as the sum of singly linked chains between the pair of tagged atoms [13]. The Ornstein-Zernike equation is appropriate for a fluid of free atoms. It is the same as Eq. (6) but without the $s$-functions. For a mixture of atoms perhaps of different concentrations, $\rho_{\alpha}$, the Ornstein-Zernike equation is

$$h_{\alpha\gamma}(r) = c_{\alpha\gamma}(r) + \sum_{\eta} \rho_{\eta} c_{\alpha\eta \star h_{\gamma\eta}(r)}. \quad (3.7)$$

On the other hand, the intramolecular correlation functions exhibited in the Chandler-Andersen equation accounts explicitly for the chemical bonding and the concomitant reduction in available configuration space. It is easily seen that the two equations are identical when the “molecules” contain only one atom, or when the atoms within a molecule are concentric.

In the Chandler-Andersen equation (or the Ornstein-Zernike equation), there are two sets of unknown functions, the $h_{\alpha\gamma}$'s and the $c_{\alpha\gamma}$'s, and one equation. Another equation is needed for closure.

The simplest closure employs the physical ideas used to construct the Chandler-Andersen equation and is applicable to the case of hard core molecules. For such molecules, by definition

$$g_{\alpha\gamma}(r) = 0, \quad r < d_{\alpha\gamma}, \quad (3.8)$$

where $d_{\alpha\gamma}$ is the distance of closest approach between atoms on different molecules. Usually, $d_{\alpha\gamma} = (s_{\alpha} + s_{\gamma})/2$ where $s_{\alpha}/2$ is the van der Waals radius of atom $\alpha$. Since we expect the $c_{\alpha\gamma}(r)$ functions to be nonzero only for distances within a range of approximately the range of intermolecular interactions, we expect approximately

$$c_{\alpha\gamma}(r) = 0, \quad r > d_{\alpha\gamma}. \quad (3.9)$$

Equations (3.6), (3.8) and (3.9) constitute a closed theory that can be used to interpret the structure of molecular fluids in terms of packing models. One must specify the bulk density, $\rho$, the intramolecular lengths which determine the $s_{\alpha\gamma}$'s and the van der Waals radii. Then the $c_{\alpha\gamma}(r)$'s are determined as that set of functions which are nonzero only for $r \leq d_{\alpha\gamma}$ and which make $g_{\alpha\gamma}(r) = 0$ for $r < d_{\alpha\gamma}$. When applied to the Ornstein-Zernike equation, i.e., when there is only one atom per molecule, this closure is the Percus-Yevick theory of hard sphere fluids [13].

Applications of the RISM theory described above have been remarkably successful in interpreting experimental studies of liquid structure. One amusing
story concerns the similarity of liquid benzene so analyzed and a bowl of breakfast cereal. It brings to mind Bernal’s ball baring model of dense fluids and amorphous solids [14].

In recent years it has become rather standard to compute pair correlation functions for liquids by straightforward computer simulations – Monte Carlo or molecular dynamics – with little thought given to the physics of the system other than the intermolecular potentials. There is nothing wrong with such calculations as they can indeed provide correct answers. But it is worth remembering that before any of these computer simulations were performed on models of molecular liquids, the structure of nonassociated liquids were well understood from the framework of the RISM theory and the underlying van der Waals perspective of the liquid state.

4. Quantum Theory by Path Ways

We now turn our attention to a remarkable mapping between quantum theory and the classical statistical mechanics of polyatomic species discussed in the preceding section. The mapping follows from Feynman’s path integral formulation of quantum mechanics [4]. Perhaps the renaissance of this approach in contemporary liquid state science began with the work of Wolynes and myself [15] where we discussed how methods such as the RISM theory and renormalization group Monte Carlo algorithms could be used in performing quantum statistical mechanical calculations. Our paper was motivated by a number of successful field theory applications performed in the 1970’s. Reference 15 provides a glimpse of this literature.

Here is the basic idea behind this approach. Consider the partition function

$$Q = \text{Tr} e^{-\beta H},$$

(4.1)

where $H$ is the Hamiltonian operator and $(k_0\beta)^{-1}$ is the temperature. The trace, $\text{Tr}$, is independent of representation, and we find it most convenient to use real configuration space, i.e., we will use the states $|x\rangle$ marking points in configuration space. This space can be multidimensional. The trace is then

$$Q = \int dx \langle x| e^{-\beta H} |x \rangle$$

(4.2)

Now, what is this object in the integrand? Recall that $\exp(-iHt/\hbar)|x\rangle$ is the state $|x, t\rangle$ that has evolved at time $t$ from the initial $|x, 0\rangle = |x\rangle$. In other words, $\exp(-iHt/\hbar)$ is the propagator for time $t$, and $\exp(-\beta H)$ is the propagator for the imaginary time $-i\beta\hbar$. The calculation of $Q$ therefore is the overlap of $|x, -i\beta\hbar\rangle$ with the initial state.
The evolution of a state can be thought of in terms of paths — in this case, quantum paths in real configuration space for imaginary time. To describe paths, we need to first analyze a step in the path. The smaller the step the simpler it is. So we will consider quantum paths as a sequence of very small steps — ultimately a continuum of infinitesimal steps. The way to brake a path into small steps is to factor the propagator into many parts,

$$e^{-\beta H} = (e^{-\beta P} P)^P.$$  \hspace{1cm} (4.3)

Thus, by inserting complete sets of states between each of the $P$ factors, we obtain

$$Q = \int dx(1) \, dx(2) \ldots \, dx(P) \langle x(1) | e^{-\epsilon H} | x(2) \rangle \langle x(2) | e^{-\epsilon H} | x(3) \rangle \ldots \langle x(P) | e^{-\epsilon H} | x(1) \rangle$$  \hspace{1cm} (4.4)

with $\epsilon = \beta / P$. We will make $P$ so large that $\epsilon$ will be very small. Further, suppose there is a natural division of $H$ into a reference part, $H_0$, and a remainder, $V(x)$. Then

$$e^{-\epsilon H} = e^{-\epsilon (H_0 + V)} = e^{-\epsilon H_0} e^{-\epsilon V} [1 + O(\epsilon^2)].$$  \hspace{1cm} (4.5)

Hence, for large enough $P$, we have the asymptotic result

$$\langle x | e^{-\epsilon H} | x' \rangle \sim \rho_0(x, x'; \epsilon) \, e^{-\epsilon V(x')}, \, \epsilon \text{ small},$$  \hspace{1cm} (4.6)

where

$$\rho_0(x, x'; \epsilon) = \langle x | e^{-\epsilon H_0} | x' \rangle$$  \hspace{1cm} (4.7)

is the unperturbed density matrix. Therefore we have

$$Q = \lim_{P \to \infty} \left[ \int dx(1) \ldots \, dx(P) \left[ \prod_{a=1}^{P} \rho_0(x(a), x(a+1); \epsilon) e^{-\epsilon V(x(a))} \right] \right]$$  \hspace{1cm} (4.8)

with the periodic or cyclic boundary condition, $x^{(P+1)} = x^{(1)}$. In the continuum limit, $P \to \infty$, the $P$-fold integrations are called “path” or “functional” integration. The integral, call it $Q_p$, has the form of a partition function for a ring “polymer” with nearest neighbor interactions. Each $x(a)$ refers to a different “time slice” for the path of the system in a configuration space.

To be a bit more explicit, let us take $H_0$ as the Hamiltonian for a collection of $N$ free particles, and $V(x) = V(r_1, r_2, \ldots, r_N)$ as the total potential energy. Then

$$\rho_0(x, x'; \epsilon) = \prod_{i=1}^{N} E(r_i, r_i'; \epsilon),$$  \hspace{1cm} (4.9)

where

$$E(r, r'; \epsilon) = \langle r | e^{-\epsilon^2/2m} | r' \rangle$$

$$= (m/2\pi \hbar^2 \epsilon)^{3/2} \exp(-m |r-r'|^2/2\hbar^2 \epsilon)$$  \hspace{1cm} (4.10)

which is a Gaussian with variance $\epsilon \hbar^2 / m$. 

Now we see that each quantum particle maps onto a ring polymer held together by Hook's law springs. The variance of each nearest neighbor spring is $\hbar^2/m$, and if unperturbed, the variance of the entire polymer or necklace would be $\beta\hbar^2/m$. The length $\lambda = (\beta\hbar^2/m)^{1/2}$ is the uncertainty spreading or thermal wave-length for a particle of mass $m$.

As a concrete illustration, Fig. 3 shows the localization of an electron in a molten salt at $T \approx 1000$ K as studied by Parrinello and Rahman [16]. The localization corresponds to the formation of a polaron [17, 18]. Notice that the polymer

Fig. 3: A sequence of electron paths (isomorphic electron polymers beginning with a non equilibrated structure and ending with a localized electron in molten K⁺Cl⁻. The paths are projected on the $x$-$y$ plane, and the ions are not shown. The side length of one of the panels is approximately 10 Å. (Adopted from Parrinello and Rahman, Ref. 16.)
structure or electron path looks very rough. It is indeed a fractal object as is indicated by its spacial scaling: the variance for the polymer with \( P \) beads is \( P \) times the variance for the nearest neighbor separation.

The \( (N!)^{-1} \) factor we are accustomed to seeing in a partition function is missing because we haven’t accounted for indistinguishability of particles. Up to this point, we are considering only the wave-like or dispersive nature of quantum theory. Symmetry and indistinguishability are features we’ll get to later.

Thus far, we see that

\[
(1 \text{ quantum particle}) \xrightarrow{\text{isomorphic mapping}} (P \rightarrow \infty \text{ classical particles})
\]

which we can represent diagrammatically as

The picture on the right looks like a diagram we would encounter in RISM theory. Indeed, it is, and one may exploit the isomorphism to good effect. The configuration space spanned by the \( P \) classical particles is the space spanned by a quantum particle obeying the uncertainty principle. As the mass \( m \) gets large, the uncertainty diminishes, the space is the same as that spanned by 1 classical particle. How big is the dispersion in space? Here are some numbers:

\[
\lambda^2 = \frac{\beta \hbar^2}{m} = 40 \text{ Å}^2 \text{ (amu) (°K)/} T m;
\]

(4.11)

thus, \( \lambda \sim 1 \) Å for He at 10 K, and \( \lambda \sim 17 \) Å for an electron at 300 K.

Now, consider indistinguishability and exchange. Imagine a two particle system. The trace of the Boltzmann operator gives the paths

\[
\frac{1}{2} \int dr_1 \int dr_2 \left[ \begin{array}{c}
\text{\includegraphics{blob1}} \\
\tau_1
\end{array} \right]
\]

where we have noted that the symmetry number for 2 identical particles is 2. But for identical particles, we also have the paths

\[
\pm \frac{1}{2} \int dr_1 \int dr_2 \left[ \begin{array}{c}
\text{\includegraphics{blob2}} \\
\tau_1
\end{array} \right]
\]
corresponding to exchange of the indistinguishable objects. Since we are to sum up all possible paths, the two particle partition function is (pictured with $P = 4$)

The "+" or "−" in the picture depends upon whether the particles are bosons or fermions, i.e., the sign of the wave function on exchange of particles. The dotted lines stand for the interparticle potentials that couple particles at equal times. Notice that if these interactions are repulsive and tend to exclude particle overlap, exchange is inhibited unless the temperature is low since then the paths can extend beyond the range of the interparticle equal time repulsions.

For fermions, notice what happens if two particles end up at the same point at the same instant. Let $\bigcirc$ denote that point. The sum of paths is then

That result is Pauli's exclusion principle. Fermion exchange leads to an alternating series for observables, and the sum over all quantum paths can be much smaller than the magnitude of the separate contributions. Thus, if fermionic exchange is frequent, the cancellation exhibited here can be problematical in straightforward numerical sampling of paths. Much current research is devoted towards developing algorithms that solve this "sign" problem, the problem of alternating weights in the Boltzmann weighted sum of quantum paths for fermionic systems.

For bosons, exchange paths add rather than subtract, and a rather spectacular effect can occur at low enough temperatures. The extent or length of a typical single particle path is then relatively long. As such, there can be a relatively small entropic cost for joining particles in exchange dimers, trimers, and so on. Indeed, one may identify a finite but low enough temperature where in the Boltzmann weighted sum over all paths, the probability of observing an $n$-mer approaches that for an $(n - 1)$-mer. This occurrence corresponds to a Bose condensation, and Feynman argued that it is the mechanism for superfluidity [19]. Recent Monte Carlo calculations by Ceperly and Pollack [20] have quantified Feynman's ideas by carrying out exactly the calculational program he prescribed. Their calcula-
tions of observables like the superfluid transition temperature for helium are in excellent agreement with experiment.

In another application of path integral quantum mechanics, Ceperley and Jacucci [21] computed the exchange probability in the fermionic solid $^3$He. For a solid, it is difficult to move atoms over distances as large as the diameter of an atom. Hence, exchange in such an environment is very unlikely and therefore infrequent. To carry out their calculation, Ceperley and Jacucci exploited the fact that the quantum amplitude for infrequent exchange is a partition function for the fleeting paths between exchange sites [15].

5. Summary

These examples, the behaviours of simple liquids, of electrons in liquids, of quantum fluids and of solids are but a few taken from the broad purviews of statistical mechanics. The consequences of Boltzmann’s $S = k_B \ln W$ and its prescribed sampling is a source of never ending fascination.

References

5. Ref. 1, 375.
CONTENTS

Preface (Otto Hitzmair) ........................................... 7
Presentation (Otto Kresten) ........................................ 9
Introduction (Giovanni Battimelli–Maria Grazia Ianniello–Otto Kresten) 13

Walter Höflechner, A Version of the Life of Ludwig Boltzmann ....... 19
Gabriele Kerber–Auguste Dick, The Dissertations prepared under the
Supervision of L. Boltzmann ........................................ 29
Adolf Hohenester, Science and the Crafts up to the Time of Boltzmann 47
Andrew D. Wilson, Boltzmann’s Philosophical Education and its Bearing on
his Mature Scientific Epistemology .................................. 57
Erhard Oeser, Boltzmann’s Epistemology and its Significance today .... 71
Salvo D’Agostino, Boltzmann and Hertz on the Bild-Conception of Physical
Theory ................................................................. 75
Anne J. Kox, Boltzmann’s Influence on H. A. Lorentz .................. 95
Maria Grazia Ianniello–Giorgio Israel, Boltzmann’s “Nachwirkung” and
Hereditary Mechanics ................................................. 113
Alfred Wehrle, Boltzmann versus Maxwell .......................... 135
Karl von Meyenn, Dynamical and Statistical Conceptions in Boltzmann’s
Physics ................................................................. 141
Dieter Flamm, Boltzmann’s Statistical Approach to Irreversibility .... 163
Otto Hitzmair, Boltzmann’s Entropy and the Concept of Information ... 175
Angelo Baracca, Boltzmann and the Foundations of Statistical Mechanics:
a Modern Appraisal .................................................. 179
Luigi Galgani, Boltzmann and the Problem of Equipartition of Energy 193
Carlo Cercignani, Resolution of the Paradoxes Related to the Boltzmann
Equation in the Light of Recent Mathematical Developments ....... 203
David Chandler, Boltzmann’s Legacy in Condensed Matter Theory: Ideas
from Van der Waals to Feynman .................................... 215
John P. Valleau, Equilibrium Ensembles and their Computer Realization:
the Gibbsian Program ................................................. 229