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Erratum: Great moments in kinetic theory: 150 years of Maxwell's (other) equations (2017 *Eur. J. Phys.* 38 065103)

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In equation (A3), an error was inadvertently introduced during the production process. The square in $\overline{\mathbf{v}\mathbf{v}}^2$ should be removed, and the corrected version of the equation is

$$\frac{\partial(nm\overline{\mathbf{v}})}{\partial t} + \nabla\cdot(nm\overline{\mathbf{v}\mathbf{v}}) - n\mathbf{F} = -n\mu\nu_m(\overline{\mathbf{v}} - \overline{\mathbf{v}}_0).$$

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Great moments in kinetic theory: 150 years of Maxwell's (other) equations

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Abstract

In 1867, just two years after laying the foundations of electromagnetism, J. Clerk Maxwell presented a fundamental paper on kinetic gas theory, in which he described the evolution of the gas in terms of certain 'moments' of its velocity distribution function. This inspired Ludwig Boltzmann to formulate his famous kinetic equation, from which followed the H-theorem and the connection with entropy. On the occasion of the 150th anniversary of publication of Maxwell's paper, we review the Maxwell–Boltzmann formalism and discuss how its generality and adaptability enable it to play a key role in describing the behaviour of a variety of systems of current interest, in both gaseous and condensed matter, and in modern-day physics and technologies which Maxwell and Boltzmann could not possibly have foreseen. In particular, we illustrate the relevance and applicability of Maxwell's formalism to the dynamic field of plasma-wakefield acceleration.

Keywords: kinetic theory, statistical mechanics, plasma-based acceleration, J Clerk Maxwell

(Some figures may appear in colour only in the online journal)

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Figure 1. Portrait of James Clerk Maxwell at Cambridge (Reprinted with permission from Emilio Segre Visual Archives).

1. Introduction

1.1. Maxwell's moment equations

J. Clerk Maxwell (pictured in figure 1) is regarded as one of the most influential physicists of all time [1–3], and his work continues to underpin many areas of modern-day scientific research and technological development.

He is best known for his equations of electromagnetism [4], but is also recognised for seminal contributions in other areas of physics, including statistical mechanics and kinetic theory. His description of transport processes through mean free path arguments [5] is standard material in basic courses on kinetic theory, as is the 'Maxwellian',

$$f_{\text{equil}}(\mathbf{v}) = n\left(\frac{m}{2\pi kT}\right)^{3/2}\exp\left(-\frac{m(\mathbf{v}-\bar{\mathbf{v}})^2}{2kT}\right), \tag{1}$$

which prescribes the distribution of velocities $\mathbf{v}$ of atoms of mass m in a gas of number density n, in *equilibrium* at absolute temperature T, and moving with an average velocity $\bar{\mathbf{v}}$. However, the most significant contribution to the field came in a paper presented to the Royal Society of London 150 years ago [6], in which he linked the microscopic world of atoms with macroscopically measurable properties, through velocity averages or 'moments' of a *non-equilibrium* velocity distribution function $f(\mathbf{r}, \mathbf{v}, t)$. In this paper, he developed 'moment equations', sometimes referred to as 'equations of change', describing the evolution of the properties of a mixture of two monatomic gases, accounting explicitly for the influence of collisions between atoms. Maxwell then obtained the equilibrium distribution function (1) as a limiting case of solution of these non-equilibrium equations, for any type of interaction between the colliding atoms. Significantly, however, it is only in the equilibrium limit that Maxwell discusses an explicit form of the distribution function.

1.2. Maxwell versus Boltzmann

It was not until some years later that Ludwig Boltzmann [7–9], inspired by Maxwell's work, provided the means of obtaining the general non-equilibrium velocity distribution function $f(\mathbf{r}, \mathbf{v}, t)$ as the solution of a kinetic equation in phase space. The procedures of Maxwell and Boltzmann, for finding the velocity moments of f, and the distribution function f itself, respectively, offer complementary ways of analysing non-equilibrium systems, and provide two of the pillars of the kinetic theory of gases. Starting with one formalism, one can arrive at the other: Maxwell's moment equations can be obtained by appropriate integration of Boltzmann kinetic equation, and conversely (but less well known) one can obtain Boltzmann's equation from the moment equations [10].

The history of the formative years of kinetic theory has been discussed by many authors (see e.g., [8, 9, 11–13]). On the other hand, the way that Maxwell's 1867 paper continues to influence modern-day physics has not received anything like the same attention, and it is the task of the present article to redress this issue.

1.3. The enduring influence of Maxwell's 'equations of matter'

There are a number of reasons why Maxwell's ideas continue to influence present-day physics:

(a) Solution of Maxwell's moment equations allows the quantities of physical interest, i.e., the velocity moments of f, to be calculated directly and efficiently, without necessarily referring to the distribution function f itself. Indeed, in the special case of interactions described by an inverse-fifth power law of force (nowadays called the 'Maxwell' model), Maxwell showed that the moment equations could be solved exactly for a non-equilibrium scenario, yielding expressions for the diffusion coefficient and other transport properties, all *without* specifying f. Stimulated by the pioneering work of Wannier for ions in gases [14], this idea has been extended to include more general forms of interaction [12], though some approximation is inevitably involved.

(b) Obtaining f from analytical or numerical solution of Boltzmann's kinetic equation may provide far more comprehensive information, but analytical solutions often only exist for highly simplified cases and numerical approaches are computationally expensive by comparison. In addition to computational economy, Maxwell's method also simplifies the mathematics and thereby promotes physical insight.

(c) Maxwell's approach also leads to empirical relations between experimentally measured quantities, that is, given data on one transport coefficient, another can be inferred directly. Thus, for example, experimental mobility coefficient data for ion swarms allows estimates of the mean ion energy and diffusion coefficients to be made, through the Wannier energy relation and generalised Einstein relations respectively [12, 14].

(d) Maxwell's procedure for gases has been extended to soft condensed matter [15] and amorphous materials [16]. Given this broad scope of applicability, we think that it is more appropriate to refer to 'Maxwell's equations of matter', rather than simply 'equations of change', as has been traditional in the gas kinetic theory literature [12].

1.4. An illustrative experiment

These ideas can be made concrete using the idealised experiment shown schematically in figure 2.

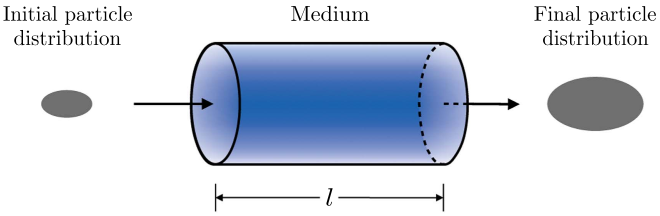

Figure 2. Schematic of an experiment to illustrate applications of Maxwell's equations of matter in both the original and modern-day contexts. The properties of a set or 'bunch' of particles change in the course of time due to gradients, external forces and interaction with the medium though which it moves, according to (4), or its relativistic generalisation (10). In Maxwell's original work [6] the particles consisted of gas atoms, and the medium was another monatomic gas. Furthermore, in a time-of-flight experiment, (4) can be applied to model a well-defined bunch of low-energy (∼few eV) charge carriers (electrons, ions, holes) as it moves a known distance l in either a gaseous medium [12, 17] or crystalline semiconductor [18]. The figure also represents plasma-wakefield acceleration experiments [19], in which a bunch of electrons is accelerated through a plasma over a distance l to highly relativistic energies (∼GeV). This can be modelled by (10).

The diagram could portray, for example, a swarm of neutral atoms, ions or electrons in a gas or plasma, positrons in a soft condensed matter medium, as in positron emission tomography, muons in a heavy hydrogen medium, as in muon catalysed fusion, or a highly relativistic electron beam in a laser-driven plasma wave. Maxwell's formalism, adapted and generalised where necessary, can be applied to these and other cases of traditional and contemporary interest.

1.5. Coupling Maxwell's equations of electromagnetism and matter

While the examples discussed in this article deal with only low density charged particles and external fields, in general charge density and currents may be sufficiently high so that self-consistent electromagnetic fields become appreciable. Then Maxwell's equations of matter are coupled with his eponymous equations for electromagnetism, as shown in figure 3. This is the situation that arises, for example, in 'fluid modelling' of plasmas [20].

1.6. About this article

Like his better known theory of the electromagnetic field, Maxwell's theory of gases continues to resonate into the twenty-first century, though often under a different guise (e.g. as 'fluid modelling' in plasma physics) and, with some notable exceptions [12], often without appropriate attribution. The 150th anniversary of the appearance of [6] provides an opportunity to confirm this important historical link, not only to enable the record to be set straight, but also to share the inspiration which we have been able to derive from this remarkable paper. In particular, we wish to establish the importance of Maxwell's formalism for systems of present-day interest, consisting of both gaseous and condensed matter, while at the same time highlighting the potential for application to new physics and technologies, which Maxwell and Boltzmann could not possibly have foreseen.

The structure of this article is as follows: we begin with a brief review of the essential elements of Maxwell's original theory of 1867 for classical gases, and then discuss the connection with Boltzmann's kinetic theory of 1872. Two contrasting examples of Maxwell's

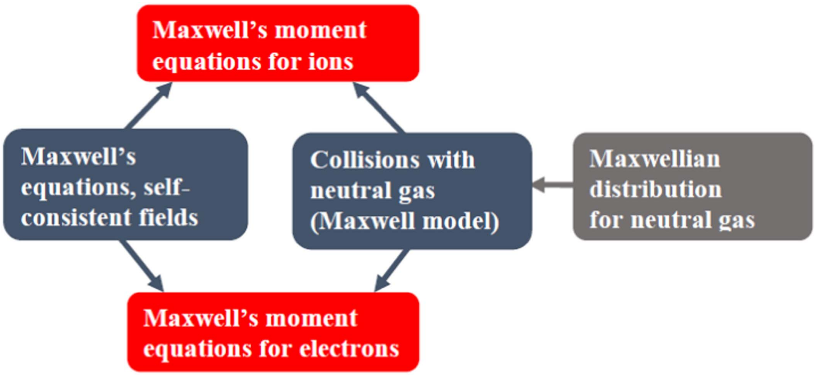

Figure 3. All elements of Maxwell's theory of both the electromagnetic field and time-evolution of matter are involved in modelling partially ionised gases and plasma. In the limit of low charged densities, the neutral gas component is approximately in equilibrium, and its velocity distribution function is the familiar 'Maxwellian', (1).

formalism are then considered in detail: firstly we explain how Maxwell's moment equations, developed originally for a model inverse-fifth power law of force, have been extended in modern times to incorporate more realistic forms of interaction. Secondly, we explain how the original approach for classical, non-relativistic particles in a gas can be extended to the relativistic electrons in a plasma accelerator. We use simple arguments stressing the basic physics and, where possible, place mathematical details in the appendices.

2. Maxwell's original theory

2.1. Velocity averages and distribution function

Consider the evolution of a group of particles moving through a background medium, as shown in figure 2. In Maxwell's original discussion, both the particles and background consisted of non-relativistic, classical monatomic gases. In the Maxwell formalism, properties of the particles are specified in terms of velocity averages or 'moments' of a non-equilibrium, space-time dependent velocity distribution function $f(\mathbf{r}, \mathbf{v}, t)$ according to

$$\overline{Q} = \frac{1}{n}\int \mathrm{d}\mathbf{v}\; Q(\mathbf{v}) f(\mathbf{r}, \mathbf{v}, t)\,, \tag{2}$$

where $Q(\mathbf{v})$ is some property of an atom, and

$$n(\mathbf{r}, t) = \int \mathrm{d}\mathbf{v}\, f(\mathbf{r}, \mathbf{v}, t)\,, \tag{3}$$

is the number density of gas atoms at position $\mathbf{r}$, time t. Setting $Q(\mathbf{v}) = m\mathbf{v}$, $Q(\mathbf{v}) = m\mathbf{v}^2/2$ etc in (2) then gives the average momentum, kinetic energy and so on. The average properties of the background gas (distinguished by a subscript '0') are similarly defined in terms of its distribution function $f_0(\mathbf{r}, \mathbf{v}_0, t)$. Note that in the Maxwell formalism, it is the moments $\overline{Q}$ in (2) which are specified, not the distribution function.

2.2. Moment equations

A general equation for $\overline{Q}$ can be derived by considering a balance between three effects:

(a) Convergence (divergence) in the flow results in an increase (decrease) of the property in the region under consideration;
(b) An external force **F** accelerates each particle, and hence causes properties of the gas to change with time;
(c) Properties change due to collisions, with the average rate of change of a property being denoted by $\overline{\partial Q/\partial t}|_{\mathrm{col}}$.

These factors are represented by the three terms on the right-hand of the balance equation,

$$\frac{\partial(n\overline{Q})}{\partial t} = -\nabla\cdot\boldsymbol{\Gamma}_Q + \frac{n}{m}\overline{\mathbf{F}\cdot\nabla_{\mathbf{v}}Q(\mathbf{v})} + n\overline{\frac{\partial Q}{\partial t}}\bigg|_{\mathrm{col}}, \tag{4}$$

where $\nabla_{\mathbf{v}}$ denotes the gradient operator in velocity space and $\boldsymbol{\Gamma}_Q = n\overline{\mathbf{v}Q}$ is the flux of property Q. Equation (4) can be derived from first principles, without any reference to the distribution function, and without specifying the detailed nature of either the particles or the background medium. Substituting $Q_0(\mathbf{v}) = 1, Q_1(\mathbf{v}) = m\mathbf{v}, Q_2(\mathbf{v}) = m\mathbf{v}^2/2$, and so forth in succession in (4) gives three general balance equations for particle number (equation of continuity), and average momentum and energy respectively. These can, in principle, be solved once the collision term is specified.

2.3. The collision term

Elastic collisions. Maxwell derived an expression for $\overline{\partial Q/\partial t}|_{\mathrm{col}}$ corresponding to elastic scattering between atoms of the gas and the background in terms of their respective velocity distribution functions f and f_0 respectively. This is written in terms of the scattering cross section σ in appendix A.

Inelastic collisions. At higher energies, when internal states of the atoms may be excited in inelastic collisions, or for molecular rather than monatomic gases, the expression for the collision term must be modified. However, the procedure for obtaining $\overline{\partial Q/\partial t}|_{\mathrm{col}}$ follows along the same lines as the case of elastic collisions [10].

Condensed matter background. Interaction terms $\overline{\partial Q/\partial t}|_{\mathrm{col}}$ have recently been developed for charge carriers in both soft condensed matter and amorphous materials, accounting for coherent scattering and trapping in localised states, respectively [15, 16]. In all cases, however, (4) provides the template for Maxwell's equations.

2.4. Relativistic electrons in a plasma medium

Charged particles such as electrons interact with a plasma medium through many-body Coulomb interactions, and finding the corresponding collision term is generally a demanding task, even more so if the electrons are relativistic. However, since the Coulomb cross section decreases rapidly with energy, highly energetic electrons in a plasma can be considered collisionless, i.e.,

$$\overline{\frac{\partial Q}{\partial t}}\bigg|_{\mathrm{col}} \approx 0\,. \tag{5}$$

The main consideration when dealing with highly energy relativistic particles is that the first two terms on the right-hand side of (4) must be modified, and momentum **p** rather than velocity, used as the independent coordinate. The corresponding Maxwell's equations will be discussed in section 4.

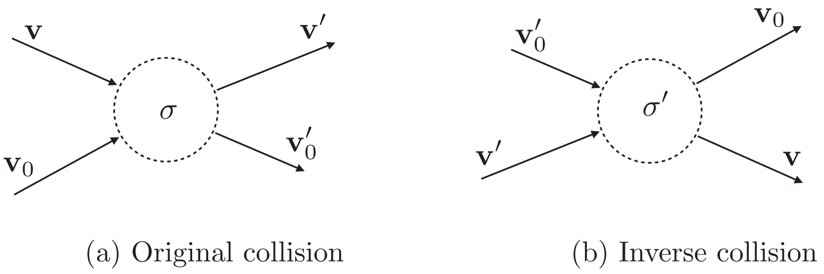

Figure 4. (a) A collision between atoms of the gas and the background medium is characterised by a differential scattering cross section σ. (b) An inverse collision, in which the roles of the incident and scattered velocities are interchanged, is characterised by a cross section σ'. Invariance of the underlying equations of motion under both the parity operation and time-reversal implies that the cross sections are identical, $\sigma' = \sigma$. For the case where the bunch and background are comprised of atoms of the same species, the equilibrium distribution function (1) can be derived from (6) (see appendix B for details).

2.5. The equilibrium distribution function

In the equilibrium state, all properties are independent of space and time, the first three members of (4) vanish, and hence

$$\left.\overline{\frac{\partial Q}{\partial t}}\right|_{\text{col}} = 0\,, \tag{6}$$

for any quantity Q. By considering the special case where the particles and the background medium constitute one and the same gas, i.e., $f = f_0$ and, by imposing time-reversal invariance on collisions (see figure 4), as Maxwell did, we can show that the solution of (6) is given by (1), for any inter-atomic interaction (see appendix B).

2.6. Maxwell model of interaction

Maxwell's expression for $\overline{\partial Q/\partial t}|_{\text{col}}$ is valid for any inter-atomic interaction potential $V(r)$, where r is the distance between atomic centres. Substituting $Q_0(\mathbf{v}) = 1$, $Q_1(\mathbf{v}) = m\mathbf{v}$, $Q_2(\mathbf{v}) = m\mathbf{v}^2/2$, $Q_3(\mathbf{v}) = m\mathbf{v}\mathbf{v}^2$ etc. successively in (4) leads to an exact, general set of moment equations which, in principle, can be solved for the quantities of interest, $\overline{Q_1}$, $\overline{Q_2}$, $\overline{Q_3}$, etc without any reference to the distribution function f. The problem is that there are always more unknowns than equations, and that the equations therefore cannot be solved without making some form of assumption or approximation. Maxwell observed that $\overline{\partial Q/\partial t}|_{\text{col}}$ simplifies significantly for an inverse-fourth power potential, $V(r) \sim r^{-4}$, and was able solve the moment equations (4) and thus obtain expressions for heat conductivity, viscosity and diffusion coefficients. Such an inverse-fifth power law of force arises from a point-charge, induced-dipole interaction, and Maxwell's model is therefore of particular relevance for modelling low-energy electron–atom and ion–atom collisions in partially ionised gases. For more general interaction potentials, it turns out that the Maxwell model still provides a reasonable first approximation to the collision terms, in a procedure known as 'momentum-transfer theory' [12].

3. Kinetic theory

3.1. Boltzmann's equation

Maxwell's work inspired Ludwig Boltzmann some six years later [7, 9, 21] to formulate a kinetic equation,

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla f + \frac{\mathbf{F}}{m} \cdot \frac{\partial f}{\partial \mathbf{v}} = \left(\frac{\partial f}{\partial t}\right)_{\text{col}}, \tag{7}$$

for the non-equilibrium velocity distribution function $f(\mathbf{r}, \mathbf{v}, t)$ itself. Boltzmann derived an expression for the collision term $(\partial f / \partial t)_{\text{col}}$ for a monatomic gas on the basis of an 'ansatz' (or postulate), which is well-documented in text books [8], but which has not been without controversy over the years. Boltzmann's famous H-theorem, and the connection with entropy and the second law of thermodynamics are also standard textbook material today. The collision term in (7) has been subsequently generalised to deal with various types of particles and their interactions in gases, plasmas and condensed matter [22].

3.2. Solution of Boltzmann's equation

Kinetic theory consists in solving Boltzmann's equation (7) for $f(\mathbf{r}, \mathbf{v}, t)$, which is then substituted in (2) to furnish the physical quantities of interest as velocity 'moments'. In contrast, Maxwell's equations yield the velocity moments directly and quickly, since there is no need to find f. However, there is a price to be paid for taking this 'short cut', since some closure approximation and loss of accuracy is inevitably involved. Solution techniques include:

(a) The Chapman–Enskog perturbative procedure for near-equilibrium situations [8].
(b) Polynomial and spherical harmonic expansion methods in velocity space for systems arbitrarily far from equilibrium [10, 12].
(c) Analytic solution of model kinetic equations [23], where the full Boltzmann collision term on the right-hand side of (7) is replaced, for example, by the Bhatnagar–Gross–Krook (BGK) relaxation time model [24].
(d) Procedures which involve discretisation of either the speed variable [25], or the velocities, (sometimes reduced to two-dimensions), as in the lattice Boltzmann equation (LBE) method [26, 27]. Since the full Boltzmann collision term is difficult to discretise, LBE is generally based on the BGK collision model [24]. While it is straightforward to replace the integral in (2) by a sum over the discrete values of f, it is otherwise difficult to make a direct comparison with the Maxwell moment method discussed here, which is based on the full Boltzmann collision term.

3.3. Relativistic kinetic equation

While Maxwell–Boltzmann kinetic theory is sufficient to deal with particles whose kinetic energy is small compared with their rest energy mc^2, modifications are necessary at higher energies, when relativistic effects are important. In the first place, the momentum $\mathbf{p} = \gamma m \mathbf{v}$ must be used in place of velocity as the fundamental coordinate, where $\gamma = \sqrt{1 + (\mathbf{p}/mc)^2} = 1\Big/\sqrt{(1 - (\mathbf{v}/c)^2)}$. The distribution function is now written as $f(\mathbf{r}, \mathbf{p}, t)$, and satisfies a kinetic equation,

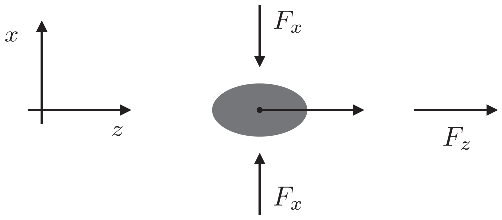

Figure 5. As an example of the experiment shown in figure 2, a beam of electrons is subject to the extreme wakefields generated in the plasma by virtue of a drive beam.

$$\frac{\partial f}{\partial t} + \frac{\mathbf{p}}{m\gamma} \cdot \nabla f + \mathbf{F} \cdot \frac{\partial f}{\partial \mathbf{p}} = \left(\frac{\partial f}{\partial t}\right)_{\text{col}}, \tag{8}$$

with an appropriately modified collision term on the right-hand side. Moments are then formed as integrals over momentum, rather than velocity, e.g., $n(\mathbf{r}, t) = \int \mathrm{d}\mathbf{p}\ f(\mathbf{r}, \mathbf{p}, t)$, and Maxwell's moment equations (4) can be reformulated in a straightforward way with a suitably modified collision term [28].

4. A modern application

4.1. Beam emittance in plasma-based accelerators

Novel methods for the acceleration of electron beams in plasmas [29–31] are attracting an ever-growing interest. This is due to the fact that plasma-based accelerators provide accelerating fields of about three orders greater than those generated with conventional techniques (see e.g. [32, 33]). This outstanding feature promises a dramatic miniaturisation of future accelerators and an according reduction of costs. Present efforts within the field of plasma-based accelerators are directed towards the generation of a large number of electrons, occupying a small (transverse) phase-space volume [34–38], and the subsequent acceleration to great energies while maintaining the populated volume [39–41]. The transverse quality of a beam is quantified by the *transverse phase-space emittance* (see e.g. [42]),

$$\epsilon = \frac{1}{mc}\sqrt{\langle x^2 \rangle \langle p_x^2 \rangle - \langle x p_x \rangle^2}, \tag{9}$$

which is a measure of the volume populated by the beam in transverse phase space, where x refers to the transverse position of an electron with respect to the beam propagation axis and p_x the momentum in the respective direction (see figure 5). The brackets denote moments over both configuration space and momentum space, in effect a generalisation of the velocity moments defined in (2). Scientists are now interested in the temporal evolution of the emittance, and the moments defining the emittance. Even if the field structure within the plasma waves is known, the evolution of the moments of the beam which is subject to these fields is not straightforward to find for arbitrary beams.

Often, particle-in-cell (PIC) simulations [43, 44] are employed for this purpose [39–41]. The PIC method offers a way to implicitly find solutions of the Boltzmann equation. This is possible by a discretisation of the phase-space distribution f in a finite number of numerical particles. These fractions of the phase-space distribution are advanced as Lagrangian particles according to the Lorentz force, i.e. along the characteristics of the Boltzmann equation. Current and charge densities of the numerical particles are deposited onto a grid on which the Maxwell's equations of electromagnetism are solved numerically. The sum of all numerical particles resembles a phase-space distribution which satisfies the Boltzmann equation. Collisions can be incorporated with a Monte-Carlo collision model [45, 46]. Despite allowing for full scale modelling on high-performance computers, PIC simulations on plasma-based accelerators are computationally highly expensive, and consume a large number of CPU hours.

4.2. Moment approach

The moment approach, although it was introduced 150 years ago, proves to be an important method in this context. Suppose now that figure 2 portrays a plasma accelerator module in which a highly relativistic beam of electrons is propagating in the fields of a plasma wave, which is generated by a high-intensity laser pulse or a high-current particle beam. The beam with known initial phase-space distribution experiences forces in transverse and longitudinal direction during the acceleration in the plasma module, as illustrated in figure 5. The aim is to compute the evolution of phase-space moments of the beam during its propagation in the plasma with high computational efficiency using the moment approach.

Since Coulomb collisions between the highly energetic electron beam and background plasma can be neglected, the electron distribution function f follows the collisionless form of (8), with the right-hand side in good approximation being zero. This allows for the formulation of an extended moment equation,

$$\frac{\partial\langle\Phi\rangle}{\partial t} = \left\langle \frac{\mathbf{p}}{m\gamma} \cdot \nabla\Phi \right\rangle + \langle \mathbf{F} \cdot \nabla_{\mathbf{p}}\Phi \rangle, \tag{10}$$

similar to (4) by multiplying the collisionless form of (8) with properties of a beam-electron, e.g. $\Phi = x^2$, $\Phi = p_x^2$ or $\Phi = xp_x$ and by integrating both over momentum space and configuration space. Instead of describing the evolution of the phase-space distribution with (8), one can now use (10) to describe the evolution of averages of the phase-space distribution, similarly as (4) describes the evolution of the velocity moments.

Generally, this approach too yields an infinite chain of moments in which each equation contains terms which depend upon higher order moments. However, in some relevant setups with a homogeneous plasma density, the transverse force is to a good approximation linear $F_x = -k_x x$. This allows for a truncation of the chain through a relatively straightforward Ansatz, leading to a finite number of coupled differential equations. These can be solved analytically, hence furnishing a fully analytical description of the emittance evolution of beams in plasma-based accelerators [47].

For more general forms of the force $\mathbf{F}(\mathbf{r}, t)$, a discretisation of the phase-space distribution $f(\mathbf{r}, \mathbf{p}, t)$ in mono-energetic subsets, located in different positions along the plasma wave is required. After employing (10) and truncating the chain of moment equations with an Ansatz, this method entails a finite number of coupled ordinary differential equations for each subset. The moments of the subsets can be found by numerically (or in specific cases analytically) solving the differential equations for each subset and subsequently combining the results in a prescribed manner to yield the overall beam averages [48].

4.3. Result from moment approach and comparison to PIC simulations

This method is used to model the emittance evolution of beams in plasma-based accelerators so as to find realistic density profiles for optimised emittance preservation. The upper plot of figure 6 shows a typical density profile (P1) and a tailored density profile obtained from a gas flow simulation of an optimised plasma cell (P2). The lower plot depicts the evolution of the

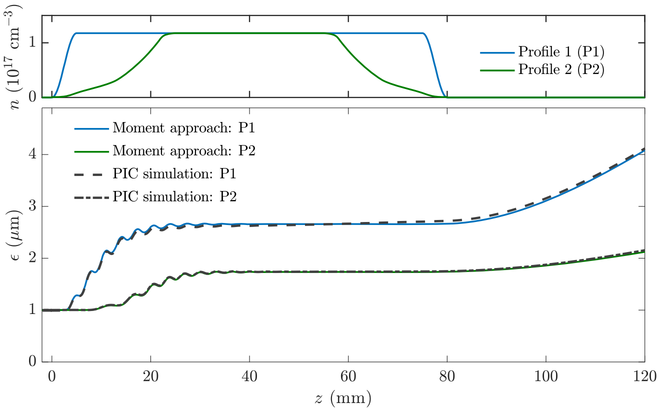

Figure 6. Evolution of the beam emittance along the modules of a plasma-based accelerator. The upper plot depicts two different plasma-electron density profiles. The lower plot shows the evolution of an accelerated electron beam as it propagates through the respective plasma profiles. Solid curves were computed using a moment approach similar to the one introduced by Maxwell [6]. The dashed and dashed–dotted curves show results of PIC simulations for the respective cases.

beam emittance for the respective profiles. The solid curves are computed using the moment approach and the dashed and dashed–dotted curves show results from PIC simulations. Figure 6 demonstrates that the results obtained with the moment approach are in excellent agreement with the PIC results (see [48] for further details).

The moment approach enables a calculation of the emittance evolution within seconds on a desktop computer while according PIC simulations consume $\sim 10^3$–10^5 CPU hours on high-performance computers. It therefore enables quick parameter scans, e.g. for the here considered emittance conservation, which are otherwise challenging and hence facilitates the advance of the plasma-based accelerator technology.

Note that modern-day simulation procedures, employing, for example, the PIC method [43, 44], effectively provide a distribution function f which satisfies the Boltzmann equation (7). Thus, figure 6, which compares results from PIC simulations with solutions obtained with equation (10), may also be taken as an indication of the level of agreement between the Maxwell and Boltzmann methods in the considered case of a relativistic electron beam. For comparison, the level of agreement for non-relativistic charged particles in gases is generally within 10% [10] (see also appendix A.4). Obtaining solutions by means of the Maxwell moment equation for specific physical cases is in general far simpler, and therefore much faster than solving Boltzmann's equation, and is also considerably less time-consuming than PIC simulations. Hence, the Maxwell method generally offers the most efficient means of obtaining the relevant quantities in such physical scenarios, i.e. the phase-space moments, without significant loss of physical accuracy.

5. Concluding remarks

J. Clerk Maxwell is regarded as one of the most influential physicists of all time, largely because of his seminal work on the equations of electromagnetism [4]. With this paper, we would like to honour one of his less well-known scientific contributions on the dynamical theory of gases [6], published exactly 150 years ago. This work continues to resonate in the modern era, sometimes without due recognition, in ways which Maxwell could not have possibly imagined. Its applicability ranges from traditional gas transport theory to present-day cutting-edge research on ultra-relativistic electron beams in plasma-wakefield accelerators. As we show, Maxwell's approach allows the quantities of physical interest to be calculated directly and extremely efficiently, without reference to the detailed distribution function f. Alternative schemes, i.e. solutions of the Boltzmann's kinetic equation for f, and PIC simulations, provide far more comprehensive information, but are computationally highly expensive. We are in no doubt that there are many more applications of Maxwell's moment formalism to come, as the technique is adapted to experiments and technologies of the future.

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Appendix A. Collision terms and Maxwell's moment equations

A.1. Maxwell's collision term

Maxwell obtained a general expression for the average rate of change of any property of the atoms of the gas under investigation due to collisions with atoms of the background gas (see figure 2). In present notation this can be written as

$$\overline{\frac{\partial Q}{\partial t}}\bigg|_{\text{col}} = \frac{1}{n}\int \mathrm{d}\mathbf{v}\, f(\mathbf{v}) \int \mathrm{d}\mathbf{v}_0 f(\mathbf{v}_0) \int_0^{\pi} \mathrm{d}\chi\ 2\pi \sin(\chi) g\sigma(g,\chi)[Q(\mathbf{v}') - Q(\mathbf{v})], \tag{A.1}$$

where primes denote post-collision properties, $g = |\mathbf{v} - \mathbf{v}_0|$ is the magnitude of the relative velocity and χ is the scattering angle in the centre-of-mass frame. The differential scattering cross section $\sigma(g, \chi)$ takes on a simple form for inter-atomic interaction potentials $V(r)$ corresponding to power laws. Thus if $V(r) \sim r^{-n}$ it can be readily shown that $\sigma(g,\chi) = \pi(\chi) g^{-4/n}$, where $\pi(\chi)$ is a function of scattering angle alone. Maxwell considered the special case of $n = 4$, for which $g\sigma(g,\chi) = \pi(\chi)$ is independent of g.

This *Maxwell model* allows the collision term to be exactly represented in a simple form, as illustrated in table A1. Here $\mu = mm_0/(m + m_0)$ is the reduced mass and an overhead bar denotes an average over velocities, as explained in the text.

A.2. Moment equations

From (4) and table A1 we obtain the equations of continuity, momentum and energy balance:

$$\frac{\partial n}{\partial t} + \nabla \cdot (n\overline{\mathbf{v}}) = 0, \tag{A.2}$$

Table A1. Collision terms for the Maxwell model, where ν_m as defined by (A.5) is a constant, and other notation is explained in the text.

Q	$\overline{\partial Q/\partial t}\vert_{\text{col}}$
1	0
$m\mathbf{v}$	$-\mu\nu_m(\overline{\mathbf{v}} - \overline{\mathbf{v}}_0)$
$m\mathbf{v}^2/2$	$-\mu\nu_m[m\overline{\mathbf{v}^2} - m_0\overline{\mathbf{v}_0^2} - (m - m_0)\overline{\mathbf{v}}\cdot\overline{\mathbf{v}}_0]/(m + m_0)$

$$\frac{\partial(nm\overline{\mathbf{v}})}{\partial t} + \nabla\cdot(nm\,\overline{\mathbf{v}\mathbf{v}^2}) - n\mathbf{F} = -n\mu\nu_m(\overline{\mathbf{v}} - \overline{\mathbf{v}}_0), \tag{A.3}$$

$$\begin{aligned}&\frac{\partial(nm\,\overline{\mathbf{v}^2}/2)}{\partial t} + \nabla\cdot(nm\overline{\mathbf{v}^2\mathbf{v}}) - n\mathbf{F}\cdot\mathbf{v}\\&\quad= -n\frac{\mu}{m + m_0}\nu_m[m\,\overline{\mathbf{v}^2} - m_0\overline{\mathbf{v}_0^2} - (m - m_0)\overline{\mathbf{v}}\cdot\overline{\mathbf{v}}_0].\end{aligned} \tag{A.4}$$

In general the collision frequency for momentum-transfer is defined by

$$\nu_m = n_0 2\pi\int_0^\pi \mathrm{d}\chi\; g\sigma(g,\chi)[1 - \cos(\chi)]\sin(\chi). \tag{A.5}$$

For the Maxwell model, where $g\sigma(g,\chi)$ is independent of g, this is a constant. Additional higher order moment equations could be added to this hierarchy if desired, as Maxwell in fact did.

A.3. Transport coefficients

Suppose that figure 2 refers to a dilute 'swarm' of ions of charge q driven through a stationary uniform gas by an electric field, that is, $\overline{\mathbf{v}}_0 = 0$, $\mathbf{F} = q\mathbf{E}$. After linearization in the spatial gradient [12], the momentum balance equation furnishes the ion particle flux,

$$\boldsymbol{\Gamma} = n\overline{\mathbf{v}} = nK\mathbf{E} - D\nabla n\,, \tag{A.6}$$

where $K = e/(\mu\nu_m)$ and $D = m\,\overline{\mathbf{v}^2}/(3\mu\nu_m)$ are ion mobility and diffusion coefficients respectively. Maxwell proceeded in a similar way to solve his set of moment equations, and thus obtained linear flux-gradient relationships for diffusion, heat and viscous flow, and expressions for the corresponding transport coefficients (diffusion, thermal conductivity and viscosity coefficients).

A.4. Beyond Maxwell's collision model

Since an inverse-fourth power law potential describes point-charge, induced-dipole interaction, Maxwell's model has proved useful for analysing charged particles (ions, electrons, positrons, muons, etc) in gases, even though it characterises only the long-range part of the actual interaction potential $V(r)$. However, in general, while $g\sigma(g,\chi)$ and hence $\nu_m(g)$ vary with g, $\overline{\partial Q/\partial t}|_{\text{col}}$ may nevertheless be approximated by expressions of the same *mathematical form* as for the Maxwell model, with ν_m replaced by an average representation of the actual collision frequency. This is the basis of so-called 'momentum-transfer theory' [12], which finds application in 'fluid modelling' of low temperature plasmas, and which furnishes transport coefficients and relations between them, such as the generalised Einstein relations, linking diffusion coefficients with mobility coefficients, and the Wannier energy relation, typically to an accuracy of around 10% [10, 12, 14, 20].

Appendix B. Equilibrium distribution function

Maxwell observed that since the equations of motion are invariant under a reversal of time, a collision and its inverse (figures 4(a) and (b) respectively) are equivalent. Thus, exchanging primed and un-primed velocities in Maxwell's original expression (appendix A), furnishes an equivalent formula for the collision term:

$$\left.\overline{\frac{\partial Q}{\partial t}}\right|_{\rm col} = \frac{1}{n}\int \mathrm{d}\mathbf{v}\; Q(\mathbf{v}) \int \mathrm{d}\mathbf{v}_0\; 2\pi \int \mathrm{d}\chi\; \sin(\chi) g\sigma(g,\,\chi)[f(\mathbf{v})f_0(\mathbf{v}_0) - f(\mathbf{v}')f_0(\mathbf{v}_0')]. \tag{B.1}$$

While Maxwell never actually wrote down this equation, he nevertheless argued along these lines, and was able to derive the equilibrium distribution function. Maxwell's procedure can be most easily illustrated for a single component gas, for which $f_0(\mathbf{v}) = f(\mathbf{v})$. As explained in the text, equilibrium prevails when $\overline{\partial Q/\partial t}|_{\rm col} = 0$. The only way that the right-hand side of (B.1) can vanish for *any* function $Q(\mathbf{v})$ is if the integrand itself vanishes for all velocities, that is particle number, if

$$f(\mathbf{v})f(\mathbf{v}_0) = f(\mathbf{v}')f(\mathbf{v}_0'). \tag{B.2}$$

Maxwell deduced that this holds if $\log(f(\mathbf{v}))$ is a linear combination of quantities conserved in a collision, that is momentum, $m\mathbf{v}$ and energy $m\mathbf{v}^2/2$. After taking the normalisation (3) into account and prescribing an absolute temperature through $m\,\overline{(\mathbf{v} - \overline{\mathbf{v}})^2}/2 = 3kT/2$, the equilibrium velocity distribution (1) follows.

The transformed collision term also leads to another important result, as explained in appendix C.

Appendix C. Maxwell's close encounter with Boltzmann's kinetic theory

Integrating Boltzmann's equation (7) with $Q(\mathbf{v})$ over all velocities furnishes Maxwell's moment equation (4), with

$$\frac{1}{n}\int \mathrm{d}\mathbf{v}\; Q(\mathbf{v})\left.\frac{\partial f}{\partial t}\right|_{\rm col} = \left.\overline{\frac{\partial Q}{\partial t}}\right|_{\rm col}. \tag{C.1}$$

Substituting the expression for Maxwell's collision term (B.1) in the right-hand side then gives

$$\int \mathrm{d}\mathbf{v}\; Q(\mathbf{v})\left.\frac{\partial f}{\partial t}\right|_{\rm col} = \int \mathrm{d}\mathbf{v}\; Q(\mathbf{v}) \int \mathrm{d}\mathbf{v}_0\; 2\pi \int \mathrm{d}\chi\; \sin(\chi) g\sigma(g,\,\chi)[f(\mathbf{v})f_0(\mathbf{v}_0) - f(\mathbf{v}')f_0(\mathbf{v}_0')]. \tag{C.2}$$

Since $Q(\mathbf{v})$ is arbitrary, the only way that this can hold is if the integrands themselves are identical, that is, if

$$\left.\frac{\partial f}{\partial t}\right|_{\rm col} = \int \mathrm{d}\mathbf{v}_0\; 2\pi,\; \int \mathrm{d}\chi\; \sin(\chi) g\sigma(g,\,\chi)[f(\mathbf{v})f_0(\mathbf{v}_0) - f(\mathbf{v}')f_0(\mathbf{v}_0')]. \tag{C.3}$$

This is precisely the kinetic collision term derived by Boltzmann [7, 21] six years *after* Maxwell's paper appeared.

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