A deterministic particle method for the Vlasov–Fokker–Planck equation in one dimension

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Received 3 August 2005; received in revised form 13 December 2006

Abstract

The Vlasov–Fokker–Planck equation is a model for a collisional, electrostatic plasma. The approximation of this equation in one spatial dimension is studied. The equation under consideration is linear in that the electric field is given as a known function that is not internally consistent with the phase space distribution function. The approximation method applied is the deterministic particle method described in Wollman and Ozizmir [Numerical approximation of the Vlasov–Poisson–Fokker–Planck system in one dimension, J. Comput. Phys. 202 (2005) 602–644]. For the present linear problem an analysis of the stability and convergence of the numerical method is carried out. In addition, computations are done that verify the convergence of the numerical solution. It is also shown that the long term asymptotics of the computed solution is in agreement with the steady state solution derived in Bouchut and Dolbeault [On long time asymptotics of the Vlasov–Fokker–Planck equation and of the Vlasov–Poisson–Fokker–Planck system with coulombic and Newtonian potentials, Differential Integral Equations 8(3) (1995) 487–514]. © 2007 Elsevier B.V. All rights reserved.

MSC: 65M06; 65M12; 65M25; 82D10

Keywords: Collisional plasma; Vlasov–Fokker–Planck equation; Deterministic particle method

1. Introduction

We consider the linear Vlasov–Fokker–Planck equation in one spatial dimension with periodic boundary conditions. That is we look for the phase space distribution function, \( f(x, v, t) \), defined on the region of phase space \( A = \{(x, v)/0 \leq x \leq L, -\infty < v < \infty\} \) that solves the initial, boundary value problem

\[
\frac{\partial f}{\partial t} + v \frac{\partial f}{\partial x} + (E(x, t) - \beta v) \frac{\partial f}{\partial v} - \beta f - q \frac{\partial^2 f}{\partial v^2} = 0,
\]

\[
f(x, v, 0) = f_0(x, v), \quad f_0(0, v) = f_0(L, v).
\] (1.1)

Here \( \beta \) and \( q \) are positive constants, and \( E \) is a known function of \( x \) and \( t \). Given the periodic boundary condition at \( t = 0 \) then the solution to (1.1) satisfies the periodic boundary condition \( f(0, v, t) = f(L, v, t) \) for \( t > 0 \). A motivation for studying (1.1) is to, in fact, solve a more complicated nonlinear problem. In this case the electric field \( E(x, t) \)
is obtained to be internally consistent with the distribution function $f$ through the solution of the Poisson equation. Thus

$$E(x, t) = -\frac{\partial \phi}{\partial x}$$

and $\phi(x, t)$ is the solution to

$$\frac{\partial^2 \phi}{\partial x^2} = -\rho(x, t),$$

$$\phi(0, t) = \phi(L, t) = 0,$$  \hspace{1cm} (1.2)

with

$$\rho(x, t) = \int_{-\infty}^{\infty} f(x, v, t) \, dv - h(x).$$

The coupled nonlinear system (1.1), (1.2) is referred to as the Vlasov–Poisson–Fokker–Planck system. This system of equations models a collisional, electrostatic plasma. In [19] a type of deterministic particle method for approximating (1.1), (1.2) is developed. This method depends on computing the solution along characteristic trajectories associated with the first order transport part of (1.1). By a transformation of variables based on the characteristic equations (1.1) is put into a form so that finite difference methods for solving parabolic type partial differential equations can be applied. In [19] we demonstrate computationally the effectiveness of the numerical method; however, no analytical results are given to guarantee the convergence. Some of the analytical problems regarding the convergence of the numerical method can be addressed by considering separately the approximation of the convection–diffusion equation (1.1) with the function $E$ given as a known external field. In the present paper we will therefore study the application of the deterministic particle method to approximate this linear problem. For this case proofs are provided on the stability and accuracy of the numerical approximation. The analysis is carried out for a somewhat simpler model problem and discretization than what is used in computation; however, numerical work is then presented to verify the convergence of the computed solution and to correlate the computational results with the analytical proofs of convergence. In addition, some computations are done to demonstrate the time asymptotic approach to the steady state. The numerical solutions show an agreement with theoretical results of Bouchut and Dolbeault [3].

Other papers on the numerical approximation of (1.1), (1.2) are [8,13,15]. These papers give deterministic methods for approximating the solution to (1.1), (1.2) which make use of characteristic curves associated with the first order transport part of (1.1). Also, random particle methods have been applied to approximate the Vlasov–Poisson–Fokker–Planck system as described in [1,7]. Another approach to approximating these equations is the Galerkin method in which the phase space distribution function is represented by a Fourier–Hermite expansion [10,11]. Some additional references on the subject are [6,9,12]. We mention that the numerical method of [19] has been generalized to the Vlasov–Poisson–Fokker–Planck system in two spatial dimensions. Some discussion of the method in two dimensions is given in [20].

2. The linear convection–diffusion equation

To put Eq. (1.1) into a different form for approximation we start with the initial value problem in all of phase space

$$\frac{\partial f}{\partial t} + v \frac{\partial f}{\partial x} + (E(x, t) - \beta v) \frac{\partial f}{\partial v} - \beta f - q \frac{\partial^2 f}{\partial v^2} = 0,$$

$$f(x, v, 0) = f_0(x, v), \quad -\infty < x < \infty, \quad -\infty < v < \infty. \hspace{1cm} (2.1)$$

In an early paper on this subject [4], Chandrasekhar approaches the problem of finding solutions to (2.1) by making a transformation of variables based on independent integrals associated with the first order transport part of the equation. Taking this approach we consider the characteristic system associated with the equation

$$\frac{\partial f}{\partial t} + v \frac{\partial f}{\partial x} + (E(x, t) - \beta v) \frac{\partial f}{\partial v} = 0.$$

\hspace{1cm} (2.2)
That is
\[
\frac{dx}{dt} = v, \quad x(0) = x_0, \tag{2.3}
\]
\[
\frac{dv}{dt} = E(x(t), t) - \beta v, \quad v(0) = v_0. \tag{2.4}
\]

The solution to (2.3), (2.4) is
\[
x(t) = x(x_0, v_0, t), \quad v(t) = v(x_0, v_0, t),
\]
continuously differentiable functions of \(x_0, v_0\) and \(t\). For each \(t\) the transformation of \(R_2\) given by
\[
(x_0, v_0) \rightarrow (x(x_0, v_0, t), v(x_0, v_0, t)) \tag{2.5}
\]
has nonzero Jacobian and is therefore invertible. Let the inverse transformation be
\[
x_0 = x_0(x, v, t), \quad v_0 = v_0(x, v, t). \tag{2.6}
\]

The functions \(x_0(x, v, t)\) and \(v_0(x, v, t)\) are independent integrals of (2.3), (2.4). As such they are each solutions to the transport equation (2.2). Under the transformation of independent variable \((x, v) \rightarrow (x_0, v_0)\) and a further change of dependent variable given by
\[
f(x_0, v_0, t) = e^{\beta t} g(x_0, v_0, t). \tag{2.1}
\]
Eq. (2.1) is put into the form
\[
\frac{\partial g}{\partial t} = q \left[ (a(x_0, v_0, t))^2 \frac{\partial^2 g}{\partial x_0^2} - 2a(x_0, v_0, t)b(x_0, v_0, t) \frac{\partial^2 g}{\partial x_0 \partial v_0} + (b(x_0, v_0, t))^2 \frac{\partial^2 g}{\partial v_0^2} 
+ c(x_0, v_0, t) \frac{\partial g}{\partial x_0} + d(x_0, v_0, t) \frac{\partial g}{\partial v_0} \right],
\]
\[
g(x_0, v_0, 0) = f_0(x_0, v_0). \tag{2.7}
\]

The coefficients in (2.7) are
\[
a(x_0, v_0, t) = e^{\beta t} \frac{\partial x}{\partial v_0}(x_0, v_0, t), \quad b(x_0, v_0, t) = e^{\beta t} \frac{\partial x}{\partial x_0}(x_0, v_0, t), \tag{2.8}
\]
\[
c(x_0, v_0, t) = e^{3\beta t} \left( \frac{\partial v}{\partial v_0} P_1 - \frac{\partial x}{\partial v_0} P_2 \right), \quad d(x_0, v_0, t) = e^{3\beta t} \left( \frac{\partial x}{\partial x_0} P_2 - \frac{\partial v}{\partial x_0} P_1 \right), \tag{2.9}
\]
where \(x(x_0, v_0, t), v(x_0, v_0, t)\) is the solution to (2.3), (2.4) and
\[
P_1 = \left[ -\frac{\partial^2 x}{\partial x_0^2} \left( \frac{\partial x}{\partial v_0} \right)^2 + 2 \frac{\partial^2 x}{\partial x_0 \partial v_0} \left( \frac{\partial x}{\partial v_0} \right) \left( \frac{\partial x}{\partial x_0} \right) - \frac{\partial^2 x}{\partial v_0^2} \left( \frac{\partial x}{\partial x_0} \right)^2 \right](x_0, v_0, t), \tag{2.10}
\]
\[
P_2 = \left[ -\frac{\partial^2 v}{\partial x_0^2} \left( \frac{\partial x}{\partial v_0} \right)^2 + 2 \frac{\partial^2 v}{\partial x_0 \partial v_0} \left( \frac{\partial x}{\partial v_0} \right) \left( \frac{\partial x}{\partial x_0} \right) - \frac{\partial^2 v}{\partial v_0^2} \left( \frac{\partial x}{\partial x_0} \right)^2 \right](x_0, v_0, t). \tag{2.11}
\]
The details of this transformation of variables are given in [19]. In terms of the solution \( g(x_0, v_0, t) \) to (2.7) the solution to (2.1) is
\[
f(x, v, t) = e^{\beta t} g(x_0(x, v, t), v_0(x, v, t), t)
\]
with \( x_0(x, v, t), v_0(x, v, t) \) defined by (2.6).

For the periodic problem (1.1) the formulation given so far is modified by assuming that \( 0 \leq x_0 \leq L \), and including the boundary condition \( g(0, v_0, t) = g(L, v_0, t) \). Also to more effectively solve (2.7) for \(-\infty < v_0 < \infty\) a further transformation of independent variable is made. Let
\[
v_0 = \frac{cu}{\sqrt{1 - u^2}}, \quad -1 < u < 1, \quad -\infty < v_0 < \infty,
\]
\[
\frac{\partial g}{\partial v_0} = \frac{1}{c}(1-u^2)^{3/2} \frac{\partial g}{\partial u},
\]
\[
\frac{\partial^2 g}{\partial v_0^2} = \frac{1}{c^2}(1-u^2)^3 \frac{\partial^2 g}{\partial u^2} - \frac{3}{c^2}(1-u^2)^2 \frac{\partial g}{\partial u}
\]
\[
= \frac{(1-u^2)^{3/2}}{c} \frac{\partial}{\partial u} \left( \frac{(1-u^2)^{3/2}}{c} \frac{\partial g}{\partial u} \right). \tag{2.12}
\]

In terms of the variables \( x_0, u, t, 0 \leq x_0 \leq L, \quad -1 < u < 1, \quad v_0(u) = cu/\sqrt{1 - u^2} \), the set of equations to be solved is
\[
\frac{\partial g}{\partial t} = q \left[ (a(x_0, v_0(u), t))^{2} \frac{\partial^2 g}{\partial x_0^2} - 2a(x_0, v_0(u), t)b(x_0, v_0(u), t)(1-u^2)^{3/2} \frac{\partial^2 g}{\partial x_0 \partial u} \right.
\]
\[
+ b(x_0, v_0(u), t) (1-u^2)^{3/2} \frac{\partial}{\partial u} \left( \frac{(1-u^2)^{3/2}}{c} \frac{\partial g}{\partial u} \right)
\]
\[
+ (b(x_0, v_0(u), t))^2 \frac{1}{c^2}(1-u^2)^3 \frac{\partial^2 g}{\partial u^2} + d(x_0, v_0(u), t) (1-u^2)^{3/2} \frac{\partial g}{\partial u} \right],
\]
\[
g(x_0, u, 0) = f_0 \left( x_0, \frac{cu}{\sqrt{1 - u^2}} \right),
\]
\[
g(0, u, t) = g(L, u, t), \quad g(x_0, -1, t) = g(x_0, 1, t) = 0. \tag{2.13}
\]

In (2.13) the coefficients are given by
\[
a(x_0, v_0(u), t) = e^{\beta t} \frac{\partial x}{\partial v_0}(x_0, v_0(u), t), \quad b(x_0, v_0(u), t) = e^{\beta t} \frac{\partial x}{\partial v_0}(x_0, v_0(u), t), \tag{2.14}
\]
\[
c(x_0, v_0(u), t) = e^{3\beta t} \left( \frac{\partial v}{\partial x_0} P_1 - \frac{\partial x}{\partial x_0} P_2 \right),
\]
\[
d(x_0, v_0(u), t) = e^{3\beta t} \left( \frac{\partial x}{\partial x_0} P_2 - \frac{\partial v}{\partial x_0} P_1 \right). \tag{2.15}
\]

Here \( x(x_0, v_0(u), t), v(x_0, v_0(u), t) \) is the solution to
\[
\frac{dx}{dt} = v, \quad x(0) = x_0, \tag{2.16}
\]
\[
\frac{dv}{dt} = E(x(x_0, v_0(u), t), t) - \beta v,
\]
\[
v(0) = v_0(u) = \frac{cu}{\sqrt{1 - u^2}} \tag{2.17}
\]
and \( P_1, P_2 \) are given by (2.10), (2.11) now regarded as functions of \( x_0, u, t \). If \( v_0 = cu/\sqrt{1-u^2} \) then \( u = u(v_0) = v_0/\sqrt{v_0^2 + c^2} \). Given the set \( A = \{ (x, v) / 0 \leq x \leq L, -\infty < v < \infty \} \) then by the periodicity (2.5) and (2.6) are regarded as transformations of \( A \) onto \( A \). The solution to \( (1.1) \) is therefore written in terms of the solution to \( (2.13) \) and the inverse transformation (2.6) as
\[
 f(x, v, t) = e^{\beta t} g(x_0(x, v, t), u(v_0(x, v, t), t)).
\] (2.18)

The functions \( a(x_0, v_0(u), t), b(x_0, v_0(u), t) \) given by (2.14) are obtained by differentiating (2.16), (2.17) and solving the resulting system of equations for the first partial derivatives as in [19, (1.28)–(1.31)]. For the coefficients \( c(x_0, v_0(u), t), d(x_0, v_0(u), t) \) as given by (2.15) it is necessary to further differentiate (2.16), (2.17) and solve a system of equations for the second partial derivatives as in [19, (1.32), (1.33)].

The solution to \( (1.1) \) can be given in terms of a sequence of solutions to \( (2.13) \). The process of developing the solution this way is the basis for the numerical approximation and is described in more detail at the beginning of Section 6.

2.1. The field-free Vlasov–Fokker–Planck equation

Some basic problems involved in computing (2.13) can be understood by considering the equations when \( E(x, t) \) is zero. For the initial value problem (2.1) the equation is now
\[
 \frac{\partial f}{\partial t} + v \frac{\partial f}{\partial x} - \beta v \frac{\partial f}{\partial v} - \beta f - q \frac{\partial^2 f}{\partial v^2} = 0,
\] (2.19)

\( f(x, v, 0) = f_0(x, v) \).

The first order equation (2.2) is
\[
 \frac{\partial f}{\partial t} + v \frac{\partial f}{\partial x} - \beta v \frac{\partial f}{\partial v} = 0.
\] (2.20)

The characteristic equations are
\[
 \frac{dx}{dt} = v, \quad x(0) = x_0,
\]
\[
 \frac{dv}{dt} = -\beta v, \quad v(0) = v_0.
\]

The solution is
\[
 x = x_0 + v_0(1 - e^{-\beta t})/\beta, \quad v = v_0e^{-\beta t}.
\] (2.21)

The inverse transformation is
\[
 x_0 = x - v(e^{\beta t} - 1)/\beta, \quad v_0 = ve^{\beta t}.
\] (2.22)

These functions of \( x, v, t \) are independent integrals of the characteristic system. In (2.7) the coefficients \( a(x_0, v_0, t), b(x_0, v_0, t) \) depend only on \( t \) and are
\[
 a(t) = e^{\beta t} \frac{\partial x}{\partial v_0} = (e^{\beta t} - 1)/\beta,
\] (2.23)
\[
 b(t) = e^{\beta t} \frac{\partial x}{\partial x_0} = e^{\beta t}.
\] (2.24)

As the second partial derivatives of (2.21) in terms of \( x_0 \) and \( v_0 \) are zero it follows that \( c(x_0, v_0, t) = 0, d(x_0, v_0, t) = 0 \). The initial value problem (2.7) is
\[
 \frac{\partial g}{\partial t} = q \left[ \left( \frac{e^{\beta t} - 1}{\beta} \right)^2 \frac{\partial^2 g}{\partial x_0^2} - 2 \left( \frac{e^{\beta t} - 1}{\beta} \right) e^{\beta t} \frac{\partial^2 g}{\partial x_0 \partial v_0} + e^{2\beta t} \frac{\partial^2 g}{\partial v_0^2} \right],
\]
\[
 g(x_0, v_0, 0) = f_0(x_0, v_0).
\] (2.25)
In terms of the solution to (2.25), the solution to (2.19) is

\[ f(x, v, t) = e^{\beta t} g \left( x - v \left( \frac{e^{\beta t} - 1}{\beta} \right), ve^{\beta t}, t \right). \]

For the periodic problem it is assumed that \( f_0(x, v) \) in (2.19) satisfies the periodic boundary condition in \( x \). With the additional transformation \( v_0 = cu/\sqrt{1 - u^2} \) then the initial-boundary value problem (2.13) is

\[
\begin{align*}
\frac{\partial g}{\partial t} &= q \left[ \left( \frac{e^{\beta t} - 1}{\beta} \right)^2 \frac{\partial^2 g}{\partial x_0^2} - 2 \left( \frac{e^{\beta t} - 1}{\beta} \right) e^{\beta t} \frac{(1 - u^2)^{3/2}}{c} \frac{\partial^2 g}{\partial x_0 \partial u} \\
&\quad + e^{2\beta t} \frac{(1 - u^2)^{3/2}}{c} \frac{\partial}{\partial u} \left( \frac{(1 - u^2)^{3/2}}{c} \frac{\partial g}{\partial u} \right) \right], \\
g(x_0, 0) &= f_0 \left( \frac{x_0}{cu}, \frac{cu}{\sqrt{1 - u^2}} \right), \\
g(0, u, t) &= g(L, u, t), \\
g(x_0, -1, t) &= g(x_0, 1, t) = 0.
\end{align*}
\]

(2.26)

From the periodicity the inverse transformation (2.22) can be written as

\[ x_0(x, v, t) = (x - v(e^{\beta t} - 1)/\beta)^*, \quad v_0(x, v, t) = ve^{\beta t}, \]

where \( (x - v(e^{\beta t} - 1)/\beta)^* = (x - v(e^{\beta t} - 1)/\beta) + mL \in [0, L] \) with \( m \) an integer. Also

\[ u(v_0(x, v, t)) = \frac{ve^{\beta t}}{\sqrt{v^2 e^{2\beta t} + c^2}}. \]

Then referring to (2.18) the solution to (2.19) with periodic boundary conditions is

\[ f(x, v, t) = e^{\beta t} g \left( (x - v(e^{\beta t} - 1)/\beta)^*, \frac{ve^{\beta t}}{\sqrt{v^2 e^{2\beta t} + c^2}}, t \right), \quad 0 \leq x \leq L, \quad -\infty < v < \infty, \]

(2.27)

where \( g(x_0, u, t) \) is the solution to (2.26).

3. Finite difference method for the field free equation

The goal is to obtain a numerical approximation to (2.19) with periodic boundary conditions. For this purpose the equation is put into the form (2.25) or (2.26). Finite difference methods are first devised that can be applied to the initial value problem in all of space, (2.25). In this case it is not too difficult to obtain some theoretical results on the stability and convergence of the methods. The numerical methods are then adapted to the initial, boundary value problem (2.26) for the purpose of computation. On an extended time interval the finite difference approximation to (2.26) is periodically reinitialized and the computation restarted on a sequence of sub-time intervals. This greatly improves the efficiency and long term stability of the numerical method. This regridding process is discussed in more detail in Section 6. We start by considering the discrete approximation of the initial value problem

\[
\begin{align*}
\frac{\partial g}{\partial t} &= q \left[ (a(t))^2 \frac{\partial^2 g}{\partial x_0^2} - 2a(t)b(t) \frac{\partial^2 g}{\partial x_0 \partial v_0} + (b(t))^2 \frac{\partial^2 g}{\partial v_0^2} \right], \\
g(x_0, v_0, 0) &= f_0(x_0, v_0).
\end{align*}
\]

(3.1)
The coefficients \(a(t), b(t)\) are continuous bounded functions. Eq. (2.25) is of the form (3.1) with \(a(t), b(t)\) given by (2.23), (2.24).

### 3.1. Forward difference method

It can be worthwhile to determine the result of applying a simple forward difference method to (3.1). Given small parameters \(\Delta x\) and \(\Delta v\) phase space is partitioned into a uniform rectangular grid \(x_0 = i \Delta x, v_0 = j \Delta v, i, j—\)integers. For the time step \(\Delta t\) then \(t_n = n \Delta t, n = 0, 1, 2, \ldots\). Let \(g(x_0, v_0, t)\) be the solution to (3.1). Then the approximation to \(g(x_0, v_0, t_n)\) is denoted \(g_{i,j}^n\). We introduce some notation. Let

\[
D_x^2 g^n_{i,j} = \frac{g^n_{i+1,j} - 2g^n_{i,j} + g^n_{i-1,j}}{(\Delta x)^2}, \quad D_v^2 g^n_{i,j} = \frac{g^n_{i,j+1} - 2g^n_{i,j} + g^n_{i,j-1}}{(\Delta v)^2},
\]

\[
D_t g^n_{i,j} = \frac{g^n_{i,j+1} - g^n_{i,j-1}}{\Delta t}, \quad D_{0,x} g^n_{i,j} = \frac{g^n_{i+1,j} - g^n_{i-1,j}}{2\Delta x}, \quad D_{0,v} g^n_{i,j} = \frac{g^n_{i,j+1} - g^n_{i,j-1}}{2\Delta v},
\]

\[
D_{0,x} D_{0,v} g^n_{i,j} = \frac{g^n_{i+1,j+1} - g^n_{i-1,j-1} - g^n_{i+1,j-1} - g^n_{i-1,j+1}}{(2\Delta x)(2\Delta v)}. \tag{3.2}
\]

In terms of the grid function \(g^n_{i,j}\) a simple forward difference approximation to (3.1) is

\[
D_t g^n_{i,j} = q[a(t_n)^2 D_x^2 g^n_{i,j} - 2a(t_n)b(t_n) D_{0,x} D_{0,v} g^n_{i,j} + b(t_n)^2 D_v^2 g^n_{i,j}],
\]

\[
g_0^n = f_0(x_0, v_0). \tag{3.3}
\]

Let \(r_1 = \Delta t/(\Delta x)^2, r_2 = \Delta t/(\Delta v)^2\) and let us define operators

\[
\delta_x^2 g^n_{i,j} = (\Delta x)^2 D_x^2 g^n_{i,j}, \quad \delta_v^2 g^n_{i,j} = (\Delta v)^2 D_v^2 g^n_{i,j},
\]

\[
\delta_{0,x} g^n_{i,j} = (2\Delta x) D_{0,x} g^n_{i,j}, \quad \delta_{0,v} g^n_{i,j} = (2\Delta v) D_{0,v} g^n_{i,j}. \tag{3.4}
\]

Then the difference equation can be written as

\[
g^{n+1}_{i,j} = g^n_{i,j} + q[a(t_n)^2 \delta_x^2 g^n_{i,j} - \frac{1}{2}a(t_n)b(t_n) \sqrt{r_1 r_2} \delta_{0,x} \delta_{0,v} g^n_{i,j} + b(t_n)^2 r_2 \delta_v^2 g^n_{i,j}]. \tag{3.5}
\]

An analysis of the stability of the difference method in the discrete \(L_2\) norm is carried out by using the discrete Fourier transform as defined in [17, p. 157]. Applying the discrete Fourier transform to Eq. (3.5) gives the equation in the transform variables \(\xi, \eta, -\pi \leq \xi, \eta \leq \pi\) of the form

\[
\hat{g}^{n+1}(\xi, \eta) = \hat{g}^n(\xi, \eta) + q[r_1 a^2 (e^{i\xi} + e^{-i\xi}) - 2 - \frac{1}{2}r_1 r_2 ab((e^{i\xi} e^{i\eta} - e^{-i\xi} e^{-i\eta}) - (e^{-i\xi} e^{i\eta} - e^{i\xi} e^{-i\eta}) + r_2 b^2 (e^{i\eta} + e^{-i\eta}) - 2)]\hat{g}^{n}(\xi, \eta).
\]

or

\[
\hat{g}^{n+1} = \hat{g}^n - 4q[r_1 a^2 \sin^2(\xi/2) - \frac{1}{2}r_1 r_2 (ab) \sin(\xi) \sin(\eta) + r_2 b^2 \sin^2(\eta/2)]\hat{g}^n.
\]

The symbol of the finite difference method is

\[
\rho(\xi, \eta) = 1 - 4q[r_1 a^2 \sin^2(\xi/2) - \frac{1}{2}r_1 r_2 (ab) \sin(\xi) \sin(\eta) + r_2 b^2 \sin^2(\eta/2)].
\]

The method is stable if \(|\rho| \leq 1\). This leads to the stability condition \(r_1 a(t_n)^2 + r_2 b(t_n)^2 \leq 1/(2q)\). Thus the forward difference method (3.3) for the initial value problem is conditionally stable. It will be assumed that \(a(t), b(t)\) are given by (2.23), (2.24). As these functions increase as \(t\) increases the restriction on \(\Delta t\) relative to \(\Delta x\) and \(\Delta v\) becomes more...
severe as time increases. The forward difference method (3.3) can be adapted to the initial, boundary value problem (2.26) and readily computed. However, as the stability condition suggests a very small time step may be required to get an accurate answer. We found this to be the case in computations done with this method.

3.2. Implicit methods

We look for methods that are stable over a long time interval with a less restrictive time step. The solution to this problem is to make the computation more implicit. Referring to the initial value problem (3.1) we determine that the following semi-implicit difference method is unconditionally stable and convergent:

\[
D_t g^{n+1} = q a(t^n) D^2_x g^n + 2 a(t^n) b(t^n) D_{0,x} D_{0,v} g^n + b(t^n) D^2_v g^n + f_0(x_0, v_0),
\]

where

\[
g^{n+1}_{i,j} = g^n_{i,j} + q a(t^n) r_1^2 \delta_x^4 g^n_{i,j} - \frac{1}{2} a(t^n) b(t^n) \sqrt{r_1 r_2} \delta_{0,x} \delta_{0,v} g^n_{i,j} + b(t^n) r_2^2 \delta_v^2 g^n_{i,j}. \tag{3.6}
\]

For vectors \( \mathbf{g} = \{g_{i,j}\} \) let \( \|g\|_{2,A} = (\sum_{i,j} |g_{i,j}|^2 \Delta x \Delta v)^{1/2} \). The linear space of vectors bounded in the norm \( \|g\|_{2,A} \) is denoted \( l_{2,A} \). The stability and convergence in the \( l_{2,A} \) norm of the difference method (3.6) is given as

**Theorem 3.1.** It is assumed that the coefficients \( a(t), b(t) \) and the solution, \( g \), of (3.1) are bounded sufficiently differentiable functions and that \( g \) and sufficient derivatives of \( g \) are bounded functions in \( L_2(R) \).

(i) The semi-implicit difference method (3.6) is unconditionally stable with respect to the \( l_{2,A} \) norm.

(ii) The solution \( \mathbf{g} = \{g_{i,j}\} \) of (3.6) converges in the \( l_{2,A} \) norm to the solution \( g(x_0, v_0, t) \) of (3.1) as \( \Delta t, \Delta x, \Delta v \to 0 \).

The accuracy of the finite difference method is \( O(\Delta t + (\Delta x)^2 + (\Delta v)^2) \).

**Proof.** Let \( r_1 = \Delta t/(\Delta x)^2, r_2 = \Delta t/(\Delta v)^2 \). Then (3.6) is written as

\[
g^{n+1}_{i,j} = g^n_{i,j} + q a(t^n) r_1^2 \delta_x^4 g^n_{i,j} - \frac{1}{2} a(t^n) b(t^n) \sqrt{r_1 r_2} \delta_{0,x} \delta_{0,v} g^n_{i,j} + b(t^n) r_2^2 \delta_v^2 g^n_{i,j}. \tag{3.7}
\]

Fourier transforming the equation according to the methods of [17] we derive that \( \hat{g}^{n+1} = \rho \hat{g}^n \) where

\[
\rho = \frac{1 + 2 q(ab) \sqrt{r_1 r_2} \sin(\xi) \sin(\eta)}{1 + 4 q a^2 r_1 \sin^2(\xi/2) + 4 q b^2 r_2 \sin^2(\eta/2)}.
\]

It can be readily determined that \( |\rho| \leq 1 \). Therefore, the difference method (3.6) is unconditionally stable.

The semi-implicit method (3.6) is also consistent. Let the difference equation (3.7) be written as

\[
L^n_{i,j}(g^n_{i,j}) = g^n_{i,j} - g^n_{i,j} - q a(t^n) r_1^2 \delta_x^4 g^n_{i,j} - \frac{1}{2} a(t^n) b(t^n) \sqrt{r_1 r_2} \delta_{0,x} \delta_{0,v} g^n_{i,j} + r_2 b(t^n) r_2^2 \delta_v^2 g^n_{i,j} = 0.
\]

Then for \( g(x_0, v_0, t) \) the solution to (3.1) and expanding in Taylor series it can be shown that

\[
L^n_{i,j}(g(x_0, v_0, t)) = \Delta t \tau^n_{i,j}, \tag{3.8}
\]

where

\[
\tau^n_{i,j} = c_1(x_0, v_0, t_n) \Delta t + c_2(x_0, v_0, t_n)(\Delta x)^2 + c_3(x_0, v_0, t_n)(\Delta v)^2.
\]

Here

\[
c_1(x_0, v_0, t_n) = \left( \frac{1}{2} \frac{\partial^2 g}{\partial t^2} - qa^2 \frac{\partial^3 g}{\partial x^2 \partial t} - qb^2 \frac{\partial^3 g}{\partial v^2 \partial t} \right)(x_0, v_0, t_n) + O(\Delta),
\]

\[
c_2(x_0, v_0, t_n) = \left( -qa^2 \frac{\partial^4 g}{\partial x^4} + \frac{1}{3} q(ab) \frac{\partial^4 g}{\partial x^3 \partial v} \right)(x_0, v_0, t_n) + O(\Delta),
\]

\[
c_3(x_0, v_0, t_n) = \left( -qb^2 \frac{\partial^4 g}{\partial v^4} + \frac{1}{3} q(ab) \frac{\partial^4 g}{\partial x \partial v^3} \right)(x_0, v_0, t_n) + O(\Delta).
\]
The quantity $O(\Delta t)$ refers to a term derived from the remainder in the Taylor formula that approaches zero as $\Delta t$, $\Delta x$, $\Delta v \to 0$. Assuming $c_1$, $c_2$, $c_3$ are bounded functions then $\tau^n_{i,j} \to 0$ as $\Delta t$, $\Delta x$, $\Delta v \to 0$ and the method is pointwise consistent.

To prove norm consistency in the discrete $L_2$ sense let us consider (3.8) in the form

$$g_{i,j}^{n+1} - qa(t_n) r_1^2 \delta^2 s_{i,j}^{n+1} - qb(t_n) r_2^2 \delta^2 s_{i,j}^{n+1} = g_{i,j}^n - \frac{1}{2} qa(t_n)b(t_n) \sqrt{r_1^2r_2^2} \delta_0 \delta_0 g_{i,j}^n + \Delta t \tau^n_{i,j}.$$  

(3.9)

We regard (3.9) as an equation of the form

$$Q_1 \bar{g}^{n+1} = Q \bar{g}^n + \Delta t \tau^n,$$  

(3.10)

where $Q_1$, $Q$ are linear operators applied to vectors $\bar{g}$, $\tau$ with components $g_{i,j}$, $\tau_{i,j}$. Then

$$\bar{g}^{n+1} = Q_1^{-1} Q \bar{g}^n + \Delta t (Q_1^{-1} \tau^n).$$

As on [17, p. 61] the discrete $L_2$, i.e., $l_{2,\Delta}$, consistency of (3.6) is proved by obtaining a bound on $\|Q_1^{-1} \tau^n\|_{2,\Delta}$ as follows:

$$\|Q_1^{-1} \tau^n\|_{2,\Delta} \leq \|Q_1^{-1}\|_{2,\Delta} \|\tau^n\|_{2,\Delta}.$$  

The operator norm for $Q_1^{-1}$ is defined as

$$\|Q_1^{-1}\|_{2,\Delta} = \sup_{\|\tau\|_{2,\Delta} = 1} \|Q_1^{-1} \tau\|_{2,\Delta}.$$  

To bound $\|Q_1^{-1}\|_{2,\Delta}$ let $\gamma$ be the symbol for $Q_1$. Then from [17, Proposition 3.1.9, p. 111] $\|Q_1^{-1}\|_{2,\Delta} \leq C$ where $C$ is a constant such that $1/\gamma \leq C$. However,

$$\gamma = 1 + 4qa^2r_1 \sin^2(\zeta/2) + 4qb^2r_2 \sin^2(\eta/2).$$

Since $1/\gamma \leq 1$ then $\|Q_1^{-1}\|_{2,\Delta} \leq 1$ and

$$\|Q_1^{-1} \tau^n\|_{2,\Delta} \leq \|\tau^n\|_{2,\Delta} \leq \|\tau\|_{2,\Delta} \Delta t + \|\bar{c}_1\|_{2,\Delta} (\Delta x)^2 + \|\bar{c}_2\|_{2,\Delta} (\Delta v)^2 + \|\bar{c}_3\|_{2,\Delta} (\Delta v)^2 \leq K (\Delta t + (\Delta x)^2 + (\Delta v)^2).$$

Assuming the functions $c_1$, $c_2$, $c_3$ are bounded in the $l_{2,\Delta}$ norm then the difference method (3.6) is norm consistent in $l_{2,\Delta}$ and accurate of order $O(\Delta t + (\Delta x)^2 + (\Delta v)^2)$. The consistency and the stability previously proved is sufficient to guarantee the convergence of the method by [17, Theorem 2.5.2, p. 79].

For the purpose of computation the semi-implicit method (3.6) is adapted to the initial, boundary value problem (2.26). In discretizing (2.26) several domains of definition are involved. Phase space is the $(x,v)$ domain given by

$$A = \{(x,v)/0 \leq x \leq L, -\infty < v < \infty\}.$$  

The $(x_0, v_0)$ domain is

$$A_0 = \{(x_0, v_0)/0 \leq x_0 \leq L, -\infty < v_0 < \infty\}$$

such that $x_0 = x_0(x, v, t)$, $v_0 = v_0(x, v, t)$ and $(x_0(x, v, t), v_0(x, v, t))$ are the functions defined by (2.6). The $(x_0, u)$ domain is

$$\Omega = \{(x_0, u)/0 \leq x_0 \leq L, -1 < u < 1\}$$

such that $v_0 = cu/\sqrt{1 - u^2}$. To approximate the solution to (2.19) in the $(x,v)$ domain we obtain a finite difference approximation to (2.26) in the $(x_0, u)$ domain.
The domain $\Omega$ is partitioned as follows: given integers $N_x, N_v$ let $\Delta x = L/N_x, \Delta u = 2/(N_v + 1)$. Then
\[ x_0 = (i - 1/2)\Delta x, \quad u_j = -1 + j\Delta u, \quad i = 1, \ldots, N_x, \quad j = 1, \ldots, N_v. \] (3.11)

Thus the region
\[ \{(x_0, u)/0 \leq x_0 \leq L, -\frac{N_v}{N_v + 1} \leq u \leq \frac{N_v}{N_v + 1}\} \subset \Omega \]
is subdivided into a uniform rectangular grid with $(x_0, u_j)$ the center of the $i, j$ rectangle on the grid. The region
\[ \{(x_0, u)/0 \leq x_0 \leq L, -1 < u < -\frac{N_v}{N_v + 1} \text{ or } \frac{N_v}{N_v + 1} < u < 1\} \]
is the part of $\Omega$ associated with points at infinity at which the distribution function is zero.

Let $v_0 = cu_j/\sqrt{1 - u_j^2}$. The point $(x_0, u_j)$ in $\Omega$ corresponds to the point $(x_0, v_0)$ in $A_0$.

For the time $T$ let $N_t$ be a positive integer and $\Delta t = T/N_t$. Then $t_n = n\Delta t, n = 0, 1, 2, \ldots, N_t$ is the partition of the time interval $[0, T]$.

The semi-implicit approximation to (2.26) is computed as follows: let
\[ s_j = \frac{(1 - u_j^2)^{3/2}}{c}, \quad s_0 = \frac{(1 - (u_j - 5\Delta u)^2)^{3/2}}{c}, \quad s_1 = \frac{(1 - (u_j + 5\Delta u)^2)^{3/2}}{c}. \] (3.12)

Adding to the notation of (3.2) an approximation to the quantity $((1 - u_j^2)^{3/2}/c)(\partial g/\partial u)(((1 - u^2)^{3/2}/c)(\partial g/\partial u))$ is given as
\[ D_0^2 g_{i,j} = s_j \left[ s_j^1 (g_{i,j+1} - g_{i,j}) - s_0^0 (g_{i,j} - g_{i,j-1}) \right] \right|_{\Delta u = s_j} \frac{[s_j^1 g_{i,j+1} - s_0^1 g_{i,j} + s_0^0 g_{i,j-1}]}{\Delta u^2}. \] (3.13)

The centered difference approximation to $((1 - u^2)^{3/2}/c)(\partial g/\partial u)$ is given as
\[ D_{0,u} g_{i,j} = s_j \frac{(g_{i,j+1} - g_{i,j-1})}{2\Delta u}. \] (3.14)

Let $g_{i,j}^0 = f_0(x_0, v_0)$, then for $n = 0, 1, 2, \ldots$ given $g_{i,j}^n$ to get $g_{i,j}^{n+1}$ we compute
\[ g_{i,j}^{n+1} = g_{i,j}^n + q\Delta t[a(t_n)]^2 D_0^2 g_{i,j}^{n+1} - 2a(t_n)b(t_n)D_{0,u} g_{i,j}^n + b(t_n)^2 D_0^2 g_{i,j}^{n+1}] . \] (3.15)

If $i = 1$ then $g_{i-1,j}^n = g_{N_x,j}^n$, if $i = N_x$ then $g_{i+1,j}^n = g_{1,j}^n$ which is the periodic boundary condition in $x_0$. If $j = 1$ then $g_{i,j-1}^n = 0$ and if $j = N_v$ then $g_{i,j+1}^n = 0$ which is the zero boundary condition at $u = \pm 1$. The coefficients $a(t), b(t)$ are given by (2.23), (2.24). We describe some methods for computing (3.15).

3.3. Iterative methods

One way to solve (3.15) for $g_{i,j}^{n+1}$ given that $g_{i,j}^n$ is known is to use an iterative procedure. Let $r_1 = \Delta t/(\Delta x)^2$, $r_2 = \Delta t/(\Delta u)^2$. If we let
\[ F_{i,j}^n = g_{i,j}^n - \frac{1}{2}q\sqrt{r_1 r_2} a(t_n) b(t_n) s_j (g_{i+1,j+1}^n - g_{i+1,j}^n - g_{i,j+1}^n + g_{i,j-1}^n) \]
and $d_j(t_n) = 1 + 2qr_1 a(t_n)^2 + qr_2 b(t_n)^2 s_j(s_j^1 + s_0^0)$ then similar to [19, (2.4)] Eq. (3.15) is written as
\[ g_{i,j}^{n+1} = \frac{q r_1 a(t_n)^2}{d_j(t_n)} (g_{i+1,j+1}^n + g_{i,j}^{n+1}) + \frac{q r_2 b(t_n)^2}{d_j(t_n)} s_j (s_j^1 g_{i,j+1}^n + s_0^0 g_{i,j-1}^n) + \frac{1}{d_j(t_n)} F_{i,j}^n. \] (3.16)
Given \( g_{i,j}^n \) Eq. (3.16) can be solved iteratively to obtain \( g_{i,j}^{n+1} \). Let \( h_{i,j}^0 = g_{i,j}^n \). Then for \( k = 0, 1, 2, \ldots \)

\[
h_{i,j}^{k+1} = \frac{q r_1 a(t_n)^2}{d_j(t_n)} (h_{i+1,j}^k + h_{i-1,j}^k) + \frac{q r_2 b(t_n)^2}{d_j(t_n)} s_j(s_j^1 h_{i,j+1}^k + s_j^0 h_{i,j-1}^k) + \frac{1}{d_j(t_n)} F_{i,j}^n.
\]  

(3.17)

This iterative procedure is referred to as the Jacobi method. Let \( \| h_k \|_{\infty,A} = \max_{i,j} | h_{i,j}^k | \) and

\[
\Theta(t_n) = \max_j \left( \frac{2 q r_1 a(t_n)^2 + q r_2 b(t_n)^2 s_j(s_j^1 + s_j^0)}{d_j(t_n)} \right).
\]

As in [19] one readily derives that

\[
\| h_{k+1} - h_k \|_{\infty,A} \leq \Theta(t_n) \| h_k - h_{k-1} \|_{\infty,A}.
\]

Since \( 0 < \Theta(t_n) < 1 \) the sequence \( \{ h_{i,j}^k \} \) converges uniformly in \( i, j \) and \( \lim_{k \to \infty} h_{i,j}^k = g_{i,j}^{n+1} \). However, as \( t \) increases the coefficients \( a(t), b(t) \) increase, and \( \Theta(t) \) gets closer to one. Thus the larger \( t \) gets the slower is the convergence of the procedure.

A more precise analysis of the convergence of (3.17) is based on the eigenvalues of the transformation so defined. Specifically, we consider the problem of finding the eigenvalues, \( \lambda \), that satisfy

\[
q r_1 a(t_n)^2 (x_i + x_{i-1}) = \lambda \frac{2 q r_1 a(t_n)^2 + q r_2 b(t_n)^2 s_j(s_j^1 + s_j^0)}{d_j(t_n)} (s_j^1 x_i + s_j^0 x_{i-1}) = \lambda x_i.
\]

(3.18)

Using separation of variables let \( h_{i,j} = x_i y_j \) then

\[
q r_1 a(t_n)^2 (x_i + x_{i-1}) = \lambda \frac{2 q r_1 a(t_n)^2 + q r_2 b(t_n)^2 s_j(s_j^1 x_i + s_j^0 x_{i-1})}{d_j(t_n)} (s_j^1 x_i + s_j^0 x_{i-1}) = \lambda x_i y_j,
\]

\[
q r_1 a(t_n)^2 \frac{(x_i + x_{i-1})}{x_i} + q r_2 b(t_n)^2 \frac{s_j(s_j^1 x_i x_j + s_j^0 x_{i-1} x_j)}{y_j} = \lambda d_j,
\]

\[
q r_1 a(t_n)^2 \frac{(x_i + x_{i-1})}{x_i} = \lambda d_j - q r_2 b(t_n)^2 \frac{s_j(s_j^1 x_i x_j + s_j^0 x_{i-1} x_j)}{y_j}.
\]

The left side of this equation is a function only of \( i \) and the right side a function only of \( j \). We therefore separately set both sides equal to a constant, \( \mu \), that is

\[
q r_1 a(t_n)^2 \frac{(x_i + x_{i-1})}{x_i} = \mu
\]

(3.19)

and

\[
\lambda d_j - q r_2 b(t_n)^2 \frac{s_j(s_j^1 x_i x_j + s_j^0 x_{i-1} x_j)}{y_j} = \mu.
\]

(3.20)

Eq. (3.19) can be solved analytically. Let

\[
\frac{(x_i + x_{i-1})}{x_i} = \alpha = \frac{\mu}{q r_1 a(t_n)^2} = \alpha
\]

or

\[
x_i + x_{i-1} = \alpha x_i.
\]
Table 1
Rates of convergence: $q = .01$

<table>
<thead>
<tr>
<th>$t_n$</th>
<th>$\lambda_{\text{max}}$</th>
<th>$\Theta(t_n)$</th>
<th>$N_{\text{itr}}$—Jacobi</th>
<th>$N_{\text{itr}}$—SOR</th>
</tr>
</thead>
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<td>0.67098</td>
<td>39</td>
<td>17</td>
</tr>
<tr>
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<td>0.82465</td>
<td>68</td>
<td>23</td>
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<td>0.92778</td>
<td>154</td>
<td>35</td>
</tr>
<tr>
<td>3</td>
<td>0.96521</td>
<td>0.96575</td>
<td>295</td>
<td>48</td>
</tr>
</tbody>
</table>

If $i = 1$, $x_i - 1 = x_N$, and if $i = N_x$, $x_i + 1 = x_1$. We therefore find the eigenvalues of the $N_x \times N_x$ matrix

$$D = \begin{pmatrix}
0 & 1 & 0 & \cdots & 0 & 0 & 1 \\
1 & 0 & 1 & \cdots & 0 & 0 & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & \cdots & 1 & 0 & 1 \\
1 & 0 & 0 & \cdots & 0 & 1 & 0 \\
\end{pmatrix}.$$  

The matrix $D$ is a circulant matrix having eigenvectors that are columns of a Fourier matrix [16, pp. 297–298]. For $k = 0, 1, \ldots, N_x - 1$ let $w^k = e^{2\pi i k/N_x}$. The eigenvalues of $D$ are readily determined to be $\lambda_k = w^{s-1} + w^{-(s-1)} = 2 \cos(2\pi(s - 1)/N_x), s = 1, \ldots, N_x$. The eigenvalues of (3.19) are therefore $\mu_s = q d s_i a x_s$. To get the eigenvalues $\lambda$ we then substitute $\mu = \mu_s$ in (3.20) and rearrange the equation to get

$$\frac{q r_2 b^2 s_j s_j^1}{d_j} y_{j+1} + \frac{\mu_s}{d_j} y_j + \frac{q r_2 b^2 s_j s_j^0}{d_j} y_{j-1} = \lambda y_j.$$  

If $j = 1, y_{j-1} = 0$ and if $j = N_v$, $y_{j+1} = 0$. To obtain $\lambda$ we therefore compute numerically the eigenvalues of the $N_v \times N_v$ matrix

$$A_s = \begin{pmatrix}
\frac{\mu_s}{d_1} & \frac{q r_2 b^2 s_1 s_1^1}{d_1} & 0 & \cdots & 0 & 0 & 0 \\
\frac{q r_2 b^2 s_2 s_2^0}{d_2} & \frac{\mu_s}{d_2} & \frac{q r_2 b^2 s_2 s_2^1}{d_2} & \cdots & 0 & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & \cdots & \frac{q r_2 b^2 s_{(N_v-1)} s_{(N_v-1)}^0}{d_{(N_v-1)}} & \frac{\mu_s}{d_{(N_v-1)}} & \frac{q r_2 b^2 s_{(N_v-1)} s_{(N_v-1)}^1}{d_{(N_v-1)}} \\
0 & 0 & 0 & \cdots & 0 & \frac{\mu_s}{d_{N_v}} & \frac{q r_2 b^2 s_N s_N^0}{d_N} \\
\end{pmatrix}$$  

(3.21)

for each $\mu_s$, $s = 1, \ldots, N_x$, $p = 1, \ldots, N_v$. The $N = N_x N_v$ eigenvalues of the transformation defined by (3.17) are denoted $\lambda_{s,p}^k$, $s = 1, \ldots, N_x$, $p = 1, \ldots, N_v$.

We are interested in finding the maximum eigenvalue, i.e., $\lambda_{\text{max}} = \max_{s,p} \lambda_{s,p}^k$. It is observed computationally that $\lambda_{\text{max}}$ is obtained when $\mu_s$ is a maximum, i.e., when $s = 1, x_1 = 1$ and $\mu_1 = 2 q a r_1$. Thus $\lambda_{\text{max}} = \max_{s,p} \lambda_{s,p}^k$, the maximum eigenvalue of the matrix (3.21) when $s = 1$. On theoretical grounds one can determine that for the Jacobi iteration $0 < \lambda_{\text{max}} < 1$, and therefore the Jacobi method converges [2, p. 111]. This is confirmed by a computation of the eigenvalues in (3.18) in which it is also observed that as $t$ increases $\lambda_{\text{max}} \to 1$, and the rate of convergence of the Jacobi method decreases. Table 1 shows the computation of $\lambda_{\text{max}}$ for the case where $L = 1$, $N_x = 100$, $N_v = 100$, $\Delta t = .01$, $q = .01$ and for $t_0 = 0, 1, 2, 3$. Also included is the number of iterations, $N_{\text{itr}}$, required for the Jacobi iteration (3.17) to converge to a tolerance of $10^{-8}$.

The method used to accelerate the convergence rate of the iterative procedure (3.17) is SOR (successive overrelaxation). Here the updated value of $h_{i,j}$ is used in the iterative procedure as soon as it is available. In addition an extrapolation is carried out based on the updated $h_{i,j}$ and its previous value. Thus for $i > 1$ and $j > 1$ instead of (3.17) we compute

$$h_{i,j}^{k+1} = \frac{q r_1 a(t_n)^2}{d_j(t_n)} (h_{i+1,j}^k + h_{i-1,j}^k) + \frac{q r_2 b(t_n)^2}{d_j(t_n)} y_j (s_j h_{i,j+1}^k + s_j h_{i,j-1}^k) + \frac{1}{d_j(t_n)} F_{i,j}^p  \quad (3.22)$$
and
\[ h_{i,j}^{k+1} = \omega \tilde{h}_{i,j}^{k+1} + (1 - \omega) h_{i,j}^k \]  
(3.23)

with \( \omega > 1 \). The problem encountered here is to determine the overrelaxation parameter, \( \omega \). Following the theory given in [2, p. 123] the optimal \( \omega \) can be determined from \( \lambda_{\text{max}} \) through the formula
\[ \omega_b = \frac{2}{1 + \sqrt{1 - j_{\text{max}}^2}}. \]

The quantity \( \lambda_{\text{max}} \) can be obtained by computing the maximum eigenvalue of \( A_x \) when \( s = 1 \). Rather than do this at each time step, \( t_n \), we determine that a good approximation to \( \lambda_{\text{max}} \) is given by \( \Theta(t_n) \). Therefore, for present purposes the optimal \( \omega \) is computed as
\[ \omega_b = \frac{2}{1 + \sqrt{1 - \Theta(t_n)^2}}. \]  
(3.24)

Included in Table 1 for the computation being considered are the values \( \Theta(t_n) \) for \( t_n = 0, 1, 2, 3 \) which can be compared to the corresponding values of \( \lambda_{\text{max}} \). Also included are the number of iterations required of the SOR algorithm, (3.22), (3.23), to converge to a tolerance of \( 10^{-8} \). By comparison with the number of iterations needed by the Jacobi method it is seen that the SOR algorithm with \( \omega_b \) given by (3.24) can substantially improve the rate of convergence of the iterative procedure.

As seen from Table 1 as \( t_n \) increases the number of iterations required by the iterative procedure increases. The regriding process described in Section 6 is a means for avoiding a large number of iterations for large \( t_n \). With regriding the semi-implicit method (3.15) is periodically reinitialized so that \( t_n = 0 \) and restarted. The solution to (2.19) is thereby computed as a sequence of solutions to (2.26). The regrid period limits the magnitude of \( t_n \) and can be chosen so that the number of iterations needed by the iterative method does not become too large.

3.4. A direct method

For relatively large values of \( q \) even with optimal acceleration of convergence and regriding a large number of iterations may be required for the iterative method. For such cases a direct method of solution of the semi-implicit procedure (3.15) may be useful. To describe a direct method first the initial value problem (3.1) is considered. Referring to (3.7) the difference equation can be written as
\[ (1 - qa(t_n)^2 r_1^2 \delta_x^2 - qb(t_n)^2 r_2^2 \delta_v^2) g_{n+1}^{i,j} = (1 - q \alpha a(t_n)b(t_n) \sqrt{r_1 r_2} \delta_{0,x} \delta_{0,v}) g_n^{i,j}. \]  
(3.25)

A modification of this equation leads to the Douglas–Rachford method as described in [17]. Let \( a = a(t_n) \), \( b = b(t_n) \) then
\[ 1 - qa^2 r_1 \delta_x^2 - qb^2 r_2 \delta_v^2 = (1 - qa^2 r_1 \delta_x^2)(1 - qb^2 r_2 \delta_v^2) - q^2 a^2 b^2 r_1 r_2 \delta_x^2 \delta_v^2. \]

Eq. (3.25) is replaced by
\[ (1 - qa^2 r_1 \delta_x^2)(1 - qb^2 r_2 \delta_v^2) g_{n+1}^{i,j} = (1 + qa^2 b^2 r_1 r_2 \delta_x^2 \delta_v^2 - \frac{1}{2} q ab \sqrt{r_1 r_2} \delta_{0,x} \delta_{0,v}) g_n^{i,j}. \]  
(3.26)

Effectively the term \( q^2 a^2 b^2 r_1 r_2 \delta_x^2 \delta_v^2 g_{n+1}^{i,j} \) is added to the left side of (3.25) and is balanced by the term \( q^2 a^2 b^2 r_1 r_2 \delta_x^2 \delta_v^2 g_n^{i,j} \) added to the right side of the equation. Eq. (3.26) is equivalent to
\[ (1 - qa^2 r_1 \delta_x^2) g_{n}^{i,j} = (1 + qb^2 r_2 \delta_v^2) g_{n+1}^{i,j} - \frac{1}{2} q ab \sqrt{r_1 r_2} \delta_{0,x} \delta_{0,v} g_{n}^{i,j}, \]  
(3.27)
\[ (1 - qb^2 r_2 \delta_v^2) g_{n+1}^{i,j} = g_{n+1}^{i,j} - qb^2 r_2 \delta_v^2 g_{n}^{i,j}. \]  
(3.28)

Thus, given \( a(t_n) \), \( b(t_n) \) and \( g_{n}^{i,j} \) at time \( t_n \), the method is to solve equation (3.27) in the index \( i \) for each \( j \) to obtain the array \( g_{n}^{i,j} \). Then solve Eq. (3.28) in the index \( j \) for each index \( i \) to obtain the array \( g_{n+1}^{i,j} \).
We prove the stability of (3.27), (3.28) as an initial value problem.

**Theorem 3.2.** Given that the coefficients \( a(t), b(t) \) of (3.1) are bounded, continuous functions the finite difference method (3.27), (3.28) is unconditionally stable with respect to the \( l_2, \lambda \) norm.

**Proof.** Fourier transforming Eqs. (3.27), (3.28) gives
\[
(1 + 4q r_1 a^2 \sin^2(\xi/2)) \hat{g}^* + (1 - 4q r_2 b^2 \sin^2(\eta/2)) \hat{g}^n + 2q ab \sqrt{r_1 r_2} \sin(\xi) \sin(\eta) \hat{g}^n = 0,
\]
\[
(1 + 4q r_2 b^2 \sin^2(\eta/2)) \hat{g}^{n+1} = \hat{g}^* + 4q r_2 b^2 \sin^2(\eta/2) \hat{g}^n.
\]
Eliminating \( \hat{g}^* \) and solving for \( \hat{g}^{n+1} \) results in
\[
\hat{g}^{n+1} = \rho \hat{g}^n
\]
where
\[
\rho = \frac{1 + 2q ab \sqrt{r_1 r_2} \sin(\xi) \sin(\eta) + 16q^2 r_1 r_2 a^2 b^2 \sin^2(\xi/2) \sin^2(\eta/2)}{(1 + 4q r_2 b^2 \sin^2(\eta/2))(1 + 4q r_1 a^2 \sin^2(\xi/2))}.
\]

It is a straightforward matter to show that \(-1 < \rho \leq 1\), and therefore the difference method (3.27), (3.28) is unconditionally stable.

We apply the Douglas–Rachford method to the initial, boundary value problem (3.15). Let \( r_1 = \Delta t/(\Delta x)^2 \), \( r_2 = \Delta t/(\Delta u)^2 \). In addition to (3.4) and referring to (3.13), (3.14) let \( \delta_{2a}^2 g_{i,j} = (\Delta u)^2 D_{u,i,j}, \delta_{0,0} g_{i,j} = (2\Delta u) D_{0,u} \). The difference equation is written as
\[
(1 - q a^2 r_1 \delta_x^2 - q b^2 r_2 \delta_u^2) g_{i,j}^{n+1} = (1 - \frac{1}{4} q ab \sqrt{r_1 r_2} \delta_{0,x} \delta_{0,u}) g_{i,j}^n.
\]
At this point the factorization proceeds exactly as before for the initial value problem to replace (3.29) with
\[
(1 - q a^2 r_1 \delta_x^2)(1 - q b^2 r_2 \delta_u^2) g_{i,j}^{n+1} = (1 + q^2 a^2 b^2 r_1 r_2 \delta_x^2 \delta_u^2 - \frac{1}{4} q ab \sqrt{r_1 r_2} \delta_{0,x} \delta_{0,u}) g_{i,j}^n
\]
or equivalently with
\[
(1 - q a^2 r_1 \delta_x^2) g_{i,j}^* = (1 + q b^2 r_2 \delta_u^2) g_{i,j}^{n+1} - \frac{1}{4} q ab \sqrt{r_1 r_2} \delta_{0,x} \delta_{0,u} g_{i,j}^n
\]
\[
(1 - q b^2 r_2 \delta_u^2) g_{i,j}^{n+1} = g_{i,j}^* - q b^2 r_2 \delta_u^2 g_{i,j}^n.
\]

The algorithm for computing (3.30), (3.31) is described in [19] (here a nonzero electric field is included). Theorem 3.2 suggests that this algorithm can be unconditionally stable, and computations indicate that this is the case. Furthermore, the efficiency of the Douglas–Rachford method is not affected by the size of the coefficients \( a(t_n), b(t_n) \). The method can be an effective means of computing a solution to (3.15) in cases where the maximum eigenvalue of the previous iterative procedure gets very close to one.

### 4. Finite difference method for nonzero electric field

If the electric field, \( E(x, t) \), in (1.1) is not zero then the coefficients in (2.13) are functions of \( x_0, u, \) and \( t \), and the finite difference approximation also includes the first partial derivative terms with coefficients \( c \) and \( d \). To develop the finite difference approximation for Eq. (2.13) we start with the initial value problem in all space given by (2.7). The analysis of our difference methods is carried out for this equation. Then, as in Section 3 the methods are adapted to the initial, boundary value problem (2.13) for the purpose of computation. As in the previous section phase space is partitioned into the uniform rectangular grid \( x_0 = l \Delta x, v_0 = j \Delta v \). The time interval is partitioned as \( t_n = n \Delta t, n = 0, 1, 2, \ldots \). The approximation to \( g(x_0, v_0, t_n) \) is denoted \( g_{i,j}^n \). It is assumed that the coefficients \( a - d \) are known functions of \( x_0, v_0, \) and \( t \). The quantities \( a(x_0, v_0, t_n) \) will be denoted \( a_{i,j}(t_n) \) and similarly for coefficients \( b - d \). The semi-implicit difference approximation for (2.7) is then given as
\[
D_x g_{i,j}^{n+1} = q [(a_{i,j}(t_n))^2 D_u^2 g_{i,j}^{n+1} - 2a_{i,j}(t_n) b_{i,j}(t_n) D_{0,x} D_{0,u} g_{i,j}^n + (b_{i,j}(t_n))^2 D_u^2 g_{i,j}^n]
+ c_{i,j}(t_n) D_{0,x} g_{i,j}^n + d_{i,j}(t_n) D_{0,u} g_{i,j}^n, \quad g_{i,j}^0 = f_0(x_0, v_0).
\]
Since the coefficients in (4.1) now depend on \( x_0 \) and \( v_0 \) one cannot easily use Fourier transform methods to analyze the stability and convergence of the finite difference approximation as was done for the field free equation. At present
we do not carry out a convergence analysis for the semi-implicit method (4.1). However, if the difference equation is fully implicit then we can provide proofs for the stability and convergence of the method. To make (4.1) into a fully implicit difference scheme one replaces $n$ with $n + 1$ in the mixed second difference term and in the terms involving first order differencing in $x$ and $v$. Also, the coefficients in the equation are evaluated at time $t_{n+1}$ rather than at time $t_n$. The fully implicit method can, in fact, be computed by an iterative procedure. We, therefore, carry out an analysis for stability and convergence of the fully implicit difference scheme. Solutions computed with this method can then be compared with those computed with the semi-implicit scheme which is the preferred method of computation. We thereby obtain some analytical verification for the computed solutions.

4.1. The fully implicit difference method

We consider the initial value problem

$$
\frac{\partial g}{\partial t} = q \left[ (a(x, v, t))^2 \frac{\partial^2 g}{\partial x^2} - 2a(x, v, t)b(x, v, t) \frac{\partial^2 g}{\partial x \partial v} + (b(x, v, t))^2 \frac{\partial^2 g}{\partial v^2} 
+ c(x, v, t) \frac{\partial g}{\partial x} + d(x, v, t) \frac{\partial g}{\partial v} \right],
$$

$$
g(x, v, 0) = f_0(x, v), \quad -\infty < x < \infty, \quad -\infty < v < \infty. \quad (4.2)
$$

To simplify notation the “0” subscript used in the previous sections is for the present dropped from $x$ and $v$. The assumption is that the solution $g(x, v, t)$ is a continuous, sufficiently differentiable and bounded function of $x$, $v$ and $t$ and that $g$ and higher derivatives as needed are bounded in $L_2(R_2)$ for each $t \in [0, T]$. The partition of phase space is then given by $x_i = i\Delta x, \ v_j = j\Delta v, \ i, j -$ integers, $g^n_{i,j}$ is the approximation to $g(x_i, v_j, t_n)$, the coefficient $a(x_i, v_j, t_n)$ is denoted $a_{i,j}(t_n)$ and similarly for the coefficients $b, c, d$. The fully implicit difference scheme for approximating (4.2) is

$$
D_t g^n_{i,j} = q[(a_{i,j}(t_{n+1}))^2 D_x g^{n+1}_{i,j} - 2a_{i,j}(t_{n+1})b_{i,j}(t_{n+1})D_{0,0}^v D_{0,v} g^{n+1}_{i,j} + (b_{i,j}(t_{n+1}))^2 D_{v,v} g^{n+1}_{i,j} 
+ c_{i,j}(t_{n+1})D_{0,0}^x D_{0,x} g^{n+1}_{i,j} + d_{i,j}(t_{n+1})D_{0,v} g^{n+1}_{i,j}], \quad g^0_{i,j} = f_0(x_i, v_j). \quad (4.3)
$$

4.1.1. Stability

The first goal is to prove the unconditional stability of the finite difference method (4.3). To motivate the proof we compute the $L_2$ norm of $g(x, v, t)$ as the solution to (4.2). Multiplying (4.2) by $g(x, v, t)$ and integrating over $x$ and $v$ then

$$
\int_{(x,v)} g \frac{\partial g}{\partial t} \, dx \, dv = q \left[ \int_{(x,v)} (a^2) g \frac{\partial^2 g}{\partial x^2} - 2(ab) g \frac{\partial^2 g}{\partial x \partial v} + (b^2) g \frac{\partial^2 g}{\partial v^2} + (c) g \frac{\partial g}{\partial v} + (d) g \frac{\partial g}{\partial v} \right] \, dv \, dx.
$$

Integrating by parts and assuming that $g(x, v, t) \to 0$ as $|x|, |v| \to \infty$ then

$$
\frac{\partial}{\partial t} \int_{(x,v)} g^2 \, dv \, dx = q \int_{(x,v)} \left( a \frac{\partial^2 (a)}{\partial x^2} - 2 \frac{\partial^2 (ab)}{\partial x \partial v} + \frac{\partial^2 (b^2)}{\partial v^2} - \frac{\partial c}{\partial x} - \frac{\partial d}{\partial v} \right) g^2 \, dv \, dx
- 2 \int_{(x,v)} \left( a \frac{\partial g}{\partial x} - b \frac{\partial g}{\partial v} \right)^2 \, dv \, dx. \quad (4.4)
$$

If the coefficients $a, c, d$ are derived according to (2.8), (2.9) one can determine that

$$
\int_{(x,v)} \left( a \frac{\partial^2 (a)}{\partial x^2} - 2 \frac{\partial^2 (ab)}{\partial x \partial v} + \frac{\partial^2 (b^2)}{\partial v^2} - \frac{\partial c}{\partial x} - \frac{\partial d}{\partial v} \right) g^2 \, dv \, dx = 0. \quad (4.5)
$$

The stability proof is given, however, for a general equation of the form (4.2), and the property (4.5) is not used. We let

$$
\int_{(x,v)} (g(x, v, t))^2 \, dv \, dx = \|g(t)\|_2^2
$$

and then compute

$$
\frac{d}{dt} \|g(t)\|_2^2 = 2 \int_{(x,v)} (g(x, v, t))^2 \frac{\partial g}{\partial t} \, dv \, dx = 2 q \int_{(x,v)} \left( a \frac{\partial^2 (a)}{\partial x^2} - 2 \frac{\partial^2 (ab)}{\partial x \partial v} + \frac{\partial^2 (b^2)}{\partial v^2} - \frac{\partial c}{\partial x} - \frac{\partial d}{\partial v} \right) (g(x, v, t))^2 \, dv \, dx
- 2 \int_{(x,v)} \left( a \frac{\partial g}{\partial x} - b \frac{\partial g}{\partial v} \right)^2 (g(x, v, t))^2 \, dv \, dx.
$$

The inequality $\|g(t)\|_2^2 \leq \|g(0)\|_2^2$ then follows from Young’s inequality and the property (4.5).
and assume the functions \( a \) and \( d \) are continuous in \( t \) and twice differentiable and bounded in \( x \) and \( v \) for each \( t \). Then

\[
\|g(t)\|_2^2 \leq \|g(0)\|_2^2 + qK \int_0^t \|g(s)\|_2^2 \, ds,
\]

where

\[
\left| \frac{\partial^2}{\partial x^2} (a^2) - 2 \frac{\partial^2}{\partial x \partial v} (ab) + \frac{\partial^2}{\partial v^2} (b^2) - \frac{\partial c}{\partial x} - \frac{\partial d}{\partial v} \right| \leq K
\]

for \( 0 \leq s \leq t \). Thus

\[
\|g(t)\|_2^2 \leq \|g(0)\|_2^2 e^{qKt} \quad \text{and} \quad \|g(t)\|_2 \leq \|g(0)\|_2 e^{qKt/2}.
\]

The unconditional stability of the finite difference method (4.3) is stated as the following theorem (an applicable definition of stability is given in [17, p. 74]).

**Theorem 4.1.** It is assumed that the coefficients \( a(x, v, t) \), \( d(x, v, t) \) of (4.2) are continuous bounded functions of \( x, v, t \) and twice differentiable in \( x \) and \( v \) for each \( t \in [0, T] \). For the solution \( g^n = \{g^n_{i,j}\} \) of (4.3) there is a constant \( K \) that depends on \( T \) such that for any \( \Delta x, \Delta v \) and for any \( \Delta t < 1/(2qK) \) then

\[
\sqrt{\sum_{i,j} (g^n_{i,j})^2} \leq (2)qKT \sqrt{\sum_{i,j} (g^0_{i,j})^2}
\]

for \( 1 \leq n \leq N_t \).

**Proof.** Eq. (4.3) is written as

\[
g^{n+1}_{i,j} = g^n_{i,j} + (\Delta t)q[(a_{i,j}(t_{n+1}))^2D_x^2g^{n+1}_{i,j} - 2a_{i,j}(t_{n+1})b_{i,j}(t_{n+1})D_0xD_0v g^{n+1}_{i,j} + (b_{i,j}(t_{n+1}))^2D_v^2g^{n+1}_{i,j} + c_{i,j}(t_{n+1})D_0xg^{n+1}_{i,j} + d_{i,j}(t_{n+1})D_0vg^{n+1}_{i,j}].
\]

(4.6)

Multiplying by \( g^{n+1}_{i,j} \) and summing over \( i, j \) then (4.6) is written as

\[
\sum_{i,j} (g^{n+1}_{i,j})^2 = \sum_{i,j} g^{n+1}_{i,j} g_{i,j} + (\Delta t)q[\text{term}1 - \text{term}2 + \text{term}3 + \text{term}4 + \text{term}5],
\]

(4.7)

where

\[
\text{term}1 = \sum_{i,j} (a_{i,j}(t_{n+1}))^2 g^{n+1}_{i,j} D_x^2 g^{n+1}_{i,j}, \quad \text{term}3 = \sum_{i,j} (b_{i,j}(t_{n+1}))^2 g^{n+1}_{i,j} D_v^2 g^{n+1}_{i,j},
\]

\[
\text{term}2 = 2 \sum_{i,j} a_{i,j}(t_{n+1})b_{i,j}(t_{n+1}) g^{n+1}_{i,j} D_0x D_0v g^{n+1}_{i,j},
\]

\[
\text{term}4 = \sum_{i,j} c_{i,j}(t_{n+1}) g^{n+1}_{i,j} D_0x g^{n+1}_{i,j}, \quad \text{term}5 = \sum_{i,j} d_{i,j}(t_{n+1}) g^{n+1}_{i,j} D_0v g^{n+1}_{i,j}.
\]

A discrete analogue of the integration by parts is carried out for each term. For the present let \( g^{n+1}_{i,j} = g_{i,j} \).
The expression obtained for term1 is a discretized version of the integration by parts for continuous functions given by
\[
\int_{(x,v)} a^2 \frac{\partial^2 g}{\partial x^2} \, dv \, dx = - \int_{(x,v)} a^2 \left( \frac{\partial g}{\partial x} \right)^2 \, dv \, dx + \frac{1}{2} \int_{(x,v)} \frac{\partial^2 (a^2)}{\partial x^2} g^2 \, dv \, dx.
\]
It can be determined that
\[
term1 = - \sum_{i,j} \left[ a^2_{i,j} (D_{0,x} g_{i,j})^2 + \frac{1}{4} (\Delta x)^2 a^2_{i,j} (D_{0,v}^2 g_{i,j})^2 \right] + \frac{1}{2} \sum_{i,j} (D_{x}^2 a^2_{i,j}) g^2_{i,j}, \quad (4.8)
\]
The derivation to arrive at (4.8) is rather lengthy; however, one can readily verify that the left side equals the right side by multiplying out squared quantities and making some change of indices in the sums. We state the expressions for the other terms in (4.7). These expressions are derived as discrete analogues of integration by parts applied to continuous functions.

\[
\begin{align*}
term2 &= - \sum_{k,j} (2ab)_{k,j} (D_{0,x} g_{k,j}) (D_{0,v} g_{k,j}) + \frac{1}{4} \sum_{i,j} (D_{x} D_{v} (2ab)_{i,j}) g_{i,j} g_{i+1,j+1} \\
&\quad + \frac{1}{4} \sum_{i,j} (D_{x} D_{v} (2ab)_{i,j-1}) g_{i,j} g_{i+1,j-1},

\text{term3} &= - \sum_{i,j} \left[ b^2_{i,j} (D_{0,v} g_{i,j})^2 + \frac{1}{4} (\Delta v)^2 b^2_{i,j} (D_{v}^2 g_{i,j})^2 \right] + \frac{1}{2} \sum_{i,j} (D_{v}^2 b^2_{i,j}) g^2_{i,j},

\text{term4} &= - \frac{1}{2} \sum_{i,j} (D_{x} c_{i,j}) g_{i,j} g_{i+1,j}, \quad \text{term5} = - \frac{1}{2} \sum_{i,j} (D_{v} d_{i,j}) g_{i,j} g_{i+1,j+1}.
\end{align*}
\]
One can verify the expressions for term2, \ldots, term5 similarly as for term1.

To continue the stability proof we refer to (4.7). With the expressions for the different terms in Eq. (4.7) can be put into the form
\[
\sum_{i,j} (g^{n+1}_{i,j})^2 = \sum_{i,j} g^{n+1}_{i,j} g^{n+1}_{i,j} + (\Delta t) q \left( - \sum_{i,j} [a_{i,j} D_{0,x} g^{n+1}_{i,j} - b_{i,j} D_{0,v} g^{n+1}_{i,j}]^2 \right. \\
&\quad - \frac{1}{4} \sum_{i,j} [(\Delta x)^2 a^2_{i,j} (D_{x}^2 g^{n+1}_{i,j})^2 + (\Delta v)^2 b^2_{i,j} (D_{v}^2 g^{n+1}_{i,j})^2] \\
&\quad + \frac{1}{2} \sum_{i,j} \left[ (D_{x}^2 a^2_{i,j}) (g^{n+1}_{i,j})^2 - \frac{1}{2} (D_{x} D_{v} (2ab)_{i,j}) g^{n+1}_{i,j} g^{n+1}_{i+1,j+1} \\
&\quad - \frac{1}{2} (D_{x} D_{v} (2ab)_{i,j-1}) g^{n+1}_{i,j} g^{n+1}_{i+1,j-1} + (D_{v}^2 b^2_{i,j}) (g^{n+1}_{i,j})^2 \\
&\quad - (D_{x} c_{i,j}) g^{n+1}_{i,j} g^{n+1}_{i+1,j} - (D_{v} d_{i,j}) g^{n+1}_{i,j} g^{n+1}_{i+1,j+1} \bigg) \right),
\]
(4.9)
We are assuming the coefficients $a, \ldots, d$ to be twice differentiable and bounded in $x$ and $v$ for each $t$. Thus, the finite differences are given the bounds
\[
|D_{x}^2 a^2_{i,j}| \leq K_1, \quad |D_{v}^2 b^2_{i,j}| \leq K_3, \quad |D_{x} D_{v} (2ab)_{i,j}| \leq K_2,
\]
\[
|D_{x} D_{v} (2ab)_{i,j-1}| \leq K_2, \quad |D_{x} c_{i,j}| \leq K_4, \quad |D_{v} d_{i,j}| \leq K_5.
\]
From (4.9) one obtains the inequality
\[
\sum_{i,j} (g_{i,j}^{n+1})^2 \leq \sum_{i,j} g_{i,j}^{n+1} g_{i,j}^n + (\Delta t) q \left( \frac{1}{2} \right) K \sum_{i,j} (g_{i,j}^{n+1})^2. \tag{4.10}
\]

Here \( K = K_1 + K_2 + K_3 + K_4 + K_5 \) and \( |g_{i,j}^{n+1} g_{i+1,j+1}^n| \leq \frac{1}{2} ((g_{i,j}^{n+1})^2 + (g_{i+1,j+1}^{n+1})^2) \) and similarly for other such products. One therefore derives the inequality
\[
\sum_{i,j} (g_{i,j}^{n+1})^2 \leq \sum_{i,j} (g_{i,j}^n)^2 + (\Delta t) q K \sum_{i,j} (g_{i,j}^{n+1})^2.
\]

Thus
\[
(1 - (\Delta t) q K) \sum_{i,j} (g_{i,j}^{n+1})^2 \leq \sum_{i,j} (g_{i,j}^n)^2.
\]

It follows that
\[
\sum_{i,j} (g_{i,j}^n)^2 \leq \frac{1}{(1 - (\Delta t) q K)} \sum_{i,j} (g_{i,j}^0)^2. \tag{4.11}
\]

To prove the unconditional stability of the finite difference method (4.3) we consider a time interval \([0, T]\) and for \( N_t \), a positive integer, let \( \frac{T}{N_t} = t, n = n \frac{T}{N_t}, n = 0, \ldots, N_t \). Also, it is assumed that the bounds \( K_1, \ldots, K_5 \) for coefficients \( a, \ldots, d \) apply for \( t \in [0, T] \). Since \( \frac{T}{N_t} < 1/(2qK) \) then
\[
\left( 1 - \frac{1}{N_t} \frac{T}{qK} \right)^{-N_t/TqK} = \left( 1 - \frac{1}{2} \right)^2 = 4.
\]

From (4.11) one then obtains the estimate
\[
\sum_{i,j} (g_{i,j}^n)^2 \leq (4)^q K T \sum_{i,j} (g_{i,j}^0)^2 \quad \text{or} \quad \sqrt{\sum_{i,j} (g_{i,j}^n)^2} \leq (2)^q K T \sqrt{\sum_{i,j} (g_{i,j}^0)^2}, \quad 1 \leq n \leq N_t. \tag{4.12}
\]

As (4.12) is independent of \( \Delta t, \Delta x, \Delta v \), assuming \( \Delta t < 1/(2qK) \), this estimate then guarantees the unconditional stability of the finite difference method (4.3). \( \square \)

We note that in the proof of Theorem 4.1 it is assumed that the coefficients \( a \ldots d \) are bounded and twice differentiable in \( x \) and \( v \). This assumption is justified by Lemma 5.2 in Section 5.

4.1.2. Consistency and convergence

The next step is to prove the consistency and convergence of the method. If we could prove consistency in the discrete \( L_2 \) sense then that would be sufficient to guarantee the convergence by [17, Theorem 2.52]. However, such a proof requires obtaining a bound on the inverse of the matrix \( Q_1 \) in an expression of the type (3.10). As the elements of the matrix depend on \( x, v \) as well as \( t \) one cannot readily apply [17, Proposition 3.1.9] as was done in Section 3 and
obtaining a bound on $\|Q^{-1}\|_{2,\Delta}$ seems difficult. Therefore, to prove the convergence we take a different approach. First, it is demonstrated that the finite difference method is pointwise consistent. Then with this result a proof of convergence in the discrete $L_2$ sense is obtained by applying the methods used in proving $L_2$ stability.

To prove pointwise consistency let $g(x, v, t)$ be the solution to (4.2) and let

$$ L(g(x_i, v_j, t_n)) = D_t g(x_i, v_j, t_n) - q[(a_{i,j}(t_{n+1}))^2 D_x^2 g(x_i, v_j, t_{n+1}) - 2a_{i,j}(t_{n+1})b_{i,j}(t_{n+1})D_{0,x} D_{0,v} g(x_i, v_j, t_{n+1}) + (b_{i,j}(t_{n+1}))^2 D_v^2 g(x_i, v_j, t_{n+1}) + c_{i,j}(t_{n+1})D_{0,x} g(x_i, v_j, t_{n+1}) + d_{i,j}(t_{n+1})D_{0,v} g(x_i, v_j, t_{n+1})]. \tag{4.13} $$

The pointwise consistency of the finite difference method (4.3) is stated as

**Proposition 4.1.** It is assumed that the solution to (4.2), $g(x, v, t)$, is a continuous, bounded, and sufficiently differentiable function of $x, v, t$. It is also assumed that there are constants $K_1, K_2$ such that $K_1 \leq \Delta x/\Delta v \leq K_2$. Then the operator $L$ defined by (4.13) has the property that $L(g(x_i, v_j, t_n)) = \tau(x_i, v_j, t_n)$ and $\tau(x_i, v_j, t_n) \to 0$ as $\Delta x, \Delta v$ and $\Delta t \to 0$.

**Proof.** Using Taylor series

$$ D_x^2 g(x_i, v_j, t_{n+1}) = \frac{\partial^2 g}{\partial x^2}(x_i, v_j, t_{n+1}) + \frac{1}{12} \frac{\partial^4 g}{\partial x^4}(x_i, v_j, t_{n+1})(\Delta x)^2 + O((\Delta x)^4), $$

where $O((\Delta x)^4)$ refers to terms obtained from the remainder in the Taylor formula. Then

$$ a_{i,j}(t_{n+1})D_x^2 g(x_i, v_j, t_{n+1}) = a_{i,j}(t_{n+1}) \frac{\partial^2 g}{\partial x^2}(x_i, v_j, t_{n+1}) + (\Delta x)^2 \left( \frac{1}{12} a_{i,j}(t_{n+1}) \frac{\partial^4 g}{\partial x^4} + O((\Delta x)^2) \right). $$

A similar expression is obtained for $b_{i,j}(t_{n+1})D_x^2 g(x_i, v_j, t_{n+1})$.

For the mixed second difference one derives

$$ D_{0,x} D_{0,v} g(x_i, v_j, t_{n+1}) = \frac{\partial^2 g}{\partial x \partial v}(x_i, v_j, t_{n+1}) + \frac{1}{6} \frac{\partial^4 g}{\partial x^3 \partial v}(\Delta x)^2 + \frac{1}{6} \frac{\partial^4 g}{\partial x \partial v^3}(\Delta v)^2 + \sum_{l=-1}^{5} O((\Delta x)^{4-l}(\Delta v)^l). $$

The assumption is that there are constants $K_1, K_2$ such that $K_1 \leq \Delta x/\Delta v \leq K_2$. With this restriction we can write

$$ \sum_{l=-1}^{5} O((\Delta x)^{4-l}(\Delta v)^l) = \sum_{l=0}^{4} O((\Delta x)^{4-l}(\Delta v)^l) $$

$$ = ((\Delta x)^2 + (\Delta v)^2)O((\Delta x)^2 + (\Delta x)(\Delta v) + (\Delta v)^2). $$

It then follows that

$$ (2ab)_{i,j}(t_{n+1})D_{0,x} D_{0,v} g(x_i, v_j, t_{n+1}) $$

$$ = (2ab)_{i,j}(t_{n+1}) \frac{\partial^2 g}{\partial x \partial v}(x_i, v_j, t_{n+1}) $$

$$ + (\Delta x)^2 \left( (2ab)_{i,j}(t_{n+1}) \frac{1}{6} \frac{\partial^4 g}{\partial x^3 \partial v} + O((\Delta x)^2 + (\Delta x)(\Delta v) + (\Delta v)^2) \right) $$

$$ + (\Delta v)^2 \left( (2ab)_{i,j}(t_{n+1}) \frac{1}{6} \frac{\partial^4 g}{\partial x \partial v^3} + O((\Delta x)^2 + (\Delta x)(\Delta v) + (\Delta v)^2) \right). $$
For the first order differences in $x$ and $v$
\[
c_{i,j}(t_{n+1})D_{0,x}g(x_i, v_j, t_{n+1}) = c_{i,j}(t_{n+1})\left(\frac{\partial g}{\partial x}(x_i, v_j, t_{n+1}) + \frac{1}{6}\frac{\partial^3 g}{\partial x^3}(x_i, v_j, t_{n+1})(\Delta x)^2 + O((\Delta x)^4)\right) = c_{i,j}(t_{n+1})\frac{\partial g}{\partial x}(x_i, v_j, t_{n+1}) + (\Delta x)^2 \left(c_{i,j}(t_{n+1})\frac{1}{6}\frac{\partial^2 g}{\partial x^2} + O((\Delta x)^2)\right).
\]

A similar expression is derive for $d_{i,j}(t_{n+1})D_{0,v}g(x_i, v_j, t_{n+1})$.

For the differencing in $t$ one has
\[
D_t g(x_i, v_j, t_n) = \frac{\partial g}{\partial t}(x_i, v_j, t_{n+1}) - \frac{1}{2}\frac{\partial^2 g}{\partial t^2}(x_i, v_j, t_{n+1})(\Delta t) + O((\Delta t)^2).
\]

Substituting the Taylor expansions for the various differenced terms in (4.13), collecting terms multiplied by $\Delta t$, $(\Delta x)^2$, $(\Delta v)^2$, and using the fact that $g(x, v, t)$ is a solution to (4.2) it now follows that
\[
L(g(x_i, v_j, t_n) = c_1(x_i, v_j, t_n)(\Delta t) + c_2(x_i, v_j, t_n)(\Delta x)^2 + c_3(x_i, v_j, t_n)(\Delta v)^2,
\]
where
\[
c_1(x_i, v_j, t_n) = -\frac{1}{2}\frac{\partial^2 g}{\partial t^2}(x_i, v_j, t_{n+1}) + O(\Delta t),
\]
\[
c_2(x_i, v_j, t_n) = q\left[-\frac{1}{12}b_{i,j}(t_{n+1})\frac{\partial^4 g}{\partial x^4} + \frac{1}{6}(2ab)_{i,j}(t_{n+1})\frac{\partial^4 g}{\partial x^2\partial v^2} - \frac{1}{6}c_{i,j}(t_{n+1})\frac{\partial^3 g}{\partial x^3} \right](x_i, v_j, t_{n+1}) + O(\Delta t),
\]
\[
c_3(x_i, v_j, t_n) = q\left[-\frac{1}{12}b_{i,j}(t_{n+1})\frac{\partial^4 g}{\partial v^4} + \frac{1}{6}(2ab)_{i,j}(t_{n+1})\frac{\partial^4 g}{\partial x^2\partial v^2} - \frac{1}{6}c_{i,j}(t_{n+1})\frac{\partial^3 g}{\partial x^3} \right](x_i, v_j, t_{n+1}) + O(\Delta t).
\]

The quantity $O(\Delta t)$ refers to terms derived from the remainder in the Taylor formula that approach zero as $\Delta x, \Delta v, \Delta t \to 0$. Let
\[
\tau(x_i, v_j, t_n) = c_1(x_i, v_j, t_n)(\Delta t) + c_2(x_i, v_j, t_n)(\Delta x)^2 + c_3(x_i, v_j, t_n)(\Delta v)^2.
\]
As $\tau(x_i, v_j, t_n) \to 0$ as $\Delta t, \Delta x, \Delta v \to 0$ then the finite difference method (4.3) is pointwise consistent. □

Using the consistency result prove the proof of stability can be adapted to prove the convergence of (4.3). Let $e_{i,j}^n = g(x_i, v_j, t_n) - g_{i,j}^n$ where $g(x, v, t)$ is the solution to (4.2) and $g_{i,j}^n$ is the solution to (4.3). For a grid function, $g_{i,j}$, we use the notation $(\sum_{i,j}(g_{i,j})^2 \Delta x \Delta v)^{1/2} = \|g\|_{2,\Delta} = \|g\|$. The convergence of the solution of (4.3) is given by

**Theorem 4.2.** It is assumed that the conditions of Theorem 4.1 and Proposition 4.1 hold. Also, it is assumed that the solution to (4.2), $g(x, v, t)$, and the necessary derivatives of $g$ are bounded functions in $L_2(R_2)$ for each $t \in [0, T]$. Then for any time $T$ there are constants $\mu(T)$ and $C(T)$ that can depend on $T$ such that for $\Delta t < \mu$
\[
\|e^n\| \leq C(T)(\Delta t + (\Delta x)^2 + (\Delta v)^2)
\]
for $0 \leq t_n \leq T$.

**Proof.** From Proposition 4.1 $L(e_{i,j}^n) = L(g(x_i, v_j, t_n) - L(g_{i,j}^n)) = \tau(x_i, v_j, t_n)$. That is
\[
D_t e_{i,j}^n - q([(a_{i,j}(t_{n+1}))^2 D_x^2 e_{i,j}^{n+1} - 2a_{i,j}(t_{n+1})b_{i,j}(t_{n+1})D_{0,x}D_{0,v}e_{i,j}^{n+1} + (b_{i,j}(t_{n+1}))^2 D_v^2 e_{i,j}^{n+1}) + c_{i,j}(t_{n+1})D_{0,x}e_{i,j}^{n+1} + d_{i,j}(t_{n+1})D_{0,v}e_{i,j}^{n+1}] = \tau(x_i, v_j, t_n)
\]
and
\[
e_{i,j}^{n+1} = e_{i,j}^n + (\Delta t)q([(a_{i,j}(t_{n+1}))^2 D_x^2 e_{i,j}^{n+1} - 2a_{i,j}(t_{n+1})b_{i,j}(t_{n+1})D_{0,x}D_{0,v}e_{i,j}^{n+1} + (b_{i,j}(t_{n+1}))^2 D_v^2 e_{i,j}^{n+1}) + c_{i,j}(t_{n+1})D_{0,x}e_{i,j}^{n+1} + d_{i,j}(t_{n+1})D_{0,v}e_{i,j}^{n+1}] + \Delta t \tau(x_i, v_j, t_n).
\]
Multiplying by $e_{i,j}^{n+1} \Delta x \Delta v$ and summing over $i, j$ one has
\[
\sum_{i,j} (e_{i,j}^{n+1})^2 \Delta x \Delta v = \sum_{i,j} e_{i,j}^{n+1} D_{x}^2 e_{i,j}^{n+1} + \Delta t s \sum_{i,j} \left[ (a_{i,j}(t_{n+1}))^2 e_{i,j}^{n+1} D_{x}^2 e_{i,j}^{n+1} - 2 a_{i,j}(t_{n+1}) b_{i,j}(t_{n+1}) e_{i,j}^{n+1} D_{0,x} D_{0,u} e_{i,j}^{n+1} + (b_{i,j}(t_{n+1}))^2 e_{i,j}^{n+1} D_{v}^2 e_{i,j}^{n+1} + c_{i,j}(t_{n+1}) e_{i,j}^{n+1} D_{0,x} e_{i,j}^{n+1} + d_{i,j}(t_{n+1}) e_{i,j}^{n+1} D_{0,u} e_{i,j}^{n+1} \right] \Delta x \Delta v + \Delta t \sum_{i,j} e_{i,j}^{n+1} \tau(x_i, v_j, t_n) \Delta x \Delta v.
\]

At this point the procedure used to prove stability can be followed starting at (4.7) and continuing to (4.10) to derive
\[
\sum_{i,j} (e_{i,j}^{n+1})^2 \Delta x \Delta v \leq \sum_{i,j} |e_{i,j}^{n+1}| e_{i,j}^{n} |\Delta x \Delta v| + \Delta t q \left( \frac{1}{2} \right) K \sum_{i,j} (e_{i,j}^{n+1})^2 \Delta x \Delta v
\]
\[
+ \Delta t \sum_{i,j} e_{i,j}^{n+1} \tau(x_i, v_j, t_n) \Delta x \Delta v.
\] (4.16)

Letting
\[
\sum_{i,j} |e_{i,j}^{n+1}| e_{i,j}^{n} |\Delta x \Delta v| \leq \frac{1}{2} (\|e^{n+1}\| + \|e^n\|)
\]
and
\[
\left| \sum_{i,j} e_{i,j}^{n+1} \tau(x_i, v_j, t_n) \Delta x \Delta v \right| \leq \|e^{n+1}\| \|\tau(\cdot, t_n)\|
\]
from (4.16) one obtains the inequality
\[
\|e^{n+1}\|^2 \leq \|e^n\|^2 + \Delta t q K \|e^{n+1}\|^2 + 2 \Delta t \|e^{n+1}\| \|\tau\|.
\] (4.17)

Now
\[
\|\tau\| = \left( \sum_{i,j} |c_1(x_i, v_j, t_n) \Delta t + c_2(x_i, v_j, t_n)(\Delta x)^2 + c_3(x_i, v_j, t_n)(\Delta v)^2 | \Delta x \Delta v \right)^{1/2}
\]
\[
\leq \Delta t \|c_1\| + (\Delta x)^2 \|c_2\| + (\Delta v)^2 \|c_3\| \leq C (\Delta t + (\Delta x)^2 + (\Delta v)^2).
\]

The constant $C$ is such that $\|c_1\|, \|c_2\|, \|c_3\| \leq C$. Here we make use of the assumptions on the boundedness of the coefficients $a, \ldots, d$ and the solution, $g$, of (4.2). Let $K_1 = K, K_2 = 2C$ then
\[
\|e^{n+1}\|^2 \leq \|e^n\|^2 + \Delta t K_1 \|e^{n+1}\|^2 + \Delta t K_2 \|e^{n+1}\| (\Delta t + (\Delta x)^2 + (\Delta v)^2).
\]
The inequality can be written as
\[
\|e^{n+1}\|^2 - \left( \frac{\Delta t K_2 (\Delta t + (\Delta x)^2 + (\Delta v)^2)}{1 - K_1 q \Delta t} \right) \|e^{n+1}\| \leq \|e^n\|^2 / (1 - K_1 q \Delta t).
\] (4.18)
Given the time interval \([0, T]\) let \(N_t\) be a positive integer, \(\Delta t = T/N_t\), and \(t_n = n\Delta t, n = 0, \ldots, N_t\). We assume \(N_t\) sufficiently large so that

\[
\Delta t < \frac{1}{2q K_1}. \tag{4.19}
\]

Thus, in the statement of the theorem \(\mu = 1/(2q K_1)\). Now \(\frac{1}{2} < 1 - \Delta t q K_1 < 1\). The inequality for \(\|e^{n+1}\|\) is obtained from (4.18) by completing the square as

\[
\left(\|e^{n+1}\| - \frac{\Delta t K_2(\Delta t + (\Delta x)^2 + (\Delta v)^2)}{2(1 - K_1 q \Delta t)} \right)^2 \leq \frac{\|e^n\|^2}{\|e^n\|^2(1 - K_1 q \Delta t)} + \left(\frac{\Delta t K_2(\Delta t + (\Delta x)^2 + (\Delta v)^2)}{2(1 - K_1 q \Delta t)} \right)^2.
\]

Thus

\[
\|e^{n+1}\| \leq \frac{\Delta t K_2(\Delta t + (\Delta x)^2 + (\Delta v)^2)}{2(1 - K_1 q \Delta t)} + \|e^n\|/\sqrt{1 - K_1 q \Delta t} + \frac{\Delta t K_2(\Delta t + (\Delta x)^2 + (\Delta v)^2)}{2(1 - K_1 q \Delta t)}.
\]

One therefore obtains the inequality

\[
\|e^{n+1}\| \leq \frac{\|e^n\|}{\sqrt{1 - K_1 q \Delta t}} + \frac{\Delta t K_2(\Delta t + (\Delta x)^2 + (\Delta v)^2)}{1 - K_1 q \Delta t}. \tag{4.20}
\]

At \(t = 0, g(x_i, v_j, 0) = g^0_{i,j} = f_0(x_i, v_j)\). Thus \(e^0_{i,j} = g(x_i, v_j, 0) - g^0_{i,j} = 0\) and \(\|e^0\| = 0\). Also \(\frac{1}{2} < 1 - K_1 q \Delta t < 1\). From the inequality (4.20) we therefore compute

\[
\|e^1\| \leq \frac{\Delta t K_2(\Delta t + (\Delta x)^2 + (\Delta v)^2)}{1 - K_1 q \Delta t}.
\]

Furthermore, if

\[
\|e^n\| \leq \frac{n \Delta t K_2(\Delta t + (\Delta x)^2 + (\Delta v)^2)}{(1 - K_1 q \Delta t)^{(n+1)/2}},
\]

then by (4.20)

\[
\|e^{n+1}\| \leq \frac{n \Delta t K_2(\Delta t + (\Delta x)^2 + (\Delta v)^2)}{(1 - K_1 q \Delta t)^{(n+1)/2}} + \frac{\Delta t K_2(\Delta t + (\Delta x)^2 + (\Delta v)^2)}{1 - K_1 q \Delta t} \leq \frac{(n + 1) \Delta t K_2(\Delta t + (\Delta x)^2 + (\Delta v)^2)}{(1 - K_1 q \Delta t)^{(n+1)/2}}.
\]

Since the inequality holds for \(n = 1\) then by induction the inequality for \(n \geq 1\) is

\[
\|e^n\| \leq \frac{n \Delta t K_2(\Delta t + (\Delta x)^2 + (\Delta v)^2)}{(1 - K_1 q \Delta t)^{(n+1)/2}}.
\]

For \(n = 0, \ldots, N_t\) then \(n \Delta t \leq T\). Thus

\[
\|e^n\| \leq \frac{T \Delta t K_2(\Delta t + (\Delta x)^2 + (\Delta v)^2)}{(1 - K_1 q \Delta t)^{(n+1)/2}} = \frac{TK_2}{(1 - K_1 q \Delta t)^{1/2}} \left(\frac{\Delta t + (\Delta x)^2 + (\Delta v)^2}{(1 - K_1 q \Delta t)^{n/2}}\right).
\]
According to (4.19) then 

\[ \| e^n \| \leq \frac{TK_3(\Delta t + (\Delta x)^2 + (\Delta v)^2)}{(1 - K_1q\Delta t)^{n/2}}. \]

Letting \( \Delta t = T/N_t \) and \( 0 \leq n \leq N_t \) the inequality is

\[ \| e^n \| \leq \frac{TK_3(\Delta t + (\Delta x)^2 + (\Delta v)^2)}{(1 - K_1q\Delta t)} \leq \frac{TK_3(\Delta t + (\Delta x)^2 + (\Delta v)^2)}{(1 - K_1qT)} \leq \frac{TK_3(\Delta t + (\Delta x)^2 + (\Delta v)^2)}{(1 - K_1qT)}^{N_t/2}. \]

Now

\[ \frac{1}{(1 - K_1qT)^{N_t/2}} = \left[ \left( 1 - \frac{1}{N_t} \frac{1}{K_1qT} \right)^{-N_t/K_1qT} \right]^{K_1qT/2}, \]

and by assumption (4.19) \( N_t/(K_1qT) > 2 \). Thus

\[ \left( 1 - \frac{1}{N_t} \frac{1}{K_1qT} \right)^{-N_t/K_1qT} < \left( 1 - \frac{1}{2} \right)^{-2} = 4 \]

so that

\[ \left[ \left( 1 - \frac{1}{N_t} \frac{1}{K_1qT} \right)^{-N_t/K_1qT} \right]^{K_1qT/2} \leq 4^{K_1qT/2} = 2^{K_1qT}. \]

We therefore obtain the inequality

\[ \| e^n \| \leq K_3T(2^{K_1qT})(\Delta t + (\Delta x)^2 + (\Delta v)^2) \]

for \( n = 0, \ldots, N_t \). As \( T \) is arbitrary the convergence of the fully implicit finite difference method (4.3) is now proved with \( C(T) = K_3T(2^{K_1qT}) \) in (4.15). The accuracy of the method is \( O(\Delta t + (\Delta x)^2 + (\Delta v)^2) \). \( \square \)

5. Difference method with approximate coefficients

In Section 4 the proof of convergence of the solution to the finite difference approximation (4.3) to the solution of the PDE (4.2) proceeds on the assumption that the coefficients \( a(x, v, t), \ldots, d(x, v, t) \) in (4.3) are known functions. However, the known function in Eq. (1.1) is the electric field, \( E(x, t) \), and the coefficients \( a, \ldots, d \) in (4.2), (4.3) are obtained according to (2.8)–(2.11) from the solution \( (x(t_0, v_0), t), (v(t_0, v_0), t)) \) to (2.3), (2.4). In an actual computation given the function \( E(x, t) \) the solution to (2.3), (2.4) and the first and second partial derivatives with respect to \( x_0 \) and \( v_0 \) are computed numerically. Hence the coefficients in (4.3) must be replaced by approximations. Therefore, we need to account for the error incurred by replacing the exact coefficients in (4.3) by approximate coefficients. We return to the previous notation in which \( (x, v) \) is a point in phase space. The transformation \( (x, v) \rightarrow (x_0, v_0) \) is defined in terms of the inverse functions (2.6). The transformation \( (x_0, v_0) \rightarrow (x_0, u) \) is defined according to (2.12). Eqs. (1.1), (2.1) are written in terms of \( (x, v) \), Eq. (2.7) in terms of \( (x_0, v_0) \), and Eq. (2.13) in terms of \( (x_0, u) \). Eq. (4.2) equates to (2.7) with coefficients \( a = -d \) given by (2.8), (2.9).

The exact particle trajectories as solutions to (2.3), (2.4) are referred to as \( (x(t_0, v_0), t), (v(t_0, v_0), t)) \). To approximate this solution the time interval \( [0, T] \) is partitioned as \( \Delta t = T/N_t, N_t \) a positive integer and \( t_n = n\Delta t, n = 0, 1, \ldots, N_t \). For the interval \( t_n \leq t \leq t_{n+1} \) the approximate trajectories with initial point \( x_0, v_0 \) given as \( (\bar{x}(t_0, v_0, t), \bar{v}(x_0, v_0, t)) \)
are obtained as solutions to
\[ \frac{d\mathbf{v}}{dt} = \mathbf{v}(t), \quad \mathbf{v}(t_n) = \mathbf{v}(x(0, v_0, t_n)). \] (5.1)

\[ \frac{d\mathbf{v}}{dt} = E(\mathbf{x}(t_n), t_n) - \beta \mathbf{v}(t), \quad \mathbf{v}(t_n) = \mathbf{v}(x(0, v_0, t_n)). \] (5.2)

The solution evaluated at \( t = t_{n+1} \) is
\[ \mathbf{x}(x(0, v_0, t_{n+1}) = \mathbf{x}(x(0, v_0, t_n) + \left( \frac{1 - e^{-\beta t}}{\beta} \right) \mathbf{v}(x(0, v_0, t_n)) \]
\[ + \left( \frac{\Delta t}{\beta} - \frac{1 - e^{-\beta \Delta t}}{\beta^2} \right) E(\mathbf{x}(x(0, v_0, t_n), t_n), t_n), \] (5.3)

\[ \mathbf{v}(x(0, v_0, t_{n+1}) = e^{-\beta \Delta t} \mathbf{v}(x(0, v_0, t_n)) + \left( \frac{1 - e^{-\beta t}}{\beta} \right) E(\mathbf{x}(x(0, v_0, t_n), t_n), t_n). \] (5.4)

The exact first partial derivatives of the functions \( (x(x(0, v_0, t), \mathbf{v}(x(0, v_0, t))) \) with respect to \( x_0 \) and \( v_0 \) are obtained as solutions to
\[ \frac{d}{dr} \left( \frac{\partial x}{\partial x_0} \right) = \frac{\partial v}{\partial x_0}, \quad \frac{\partial x}{\partial x_0}(0) = 1, \] (5.5)

\[ \frac{d}{dr} \left( \frac{\partial v}{\partial x_0} \right) = \frac{\partial E}{\partial x_0}(x(x_0, v_0, t), t) \left( \frac{\partial x}{\partial x_0} \right) - \beta \left( \frac{\partial v}{\partial x_0} \right), \quad \frac{\partial v}{\partial x_0}(0) = 0 \] (5.6)

and
\[ \frac{d}{dr} \left( \frac{\partial x}{\partial v_0} \right) = \frac{\partial v}{\partial v_0}, \quad \frac{\partial x}{\partial v_0}(0) = 0. \] (5.7)

\[ \frac{d}{dr} \left( \frac{\partial v}{\partial v_0} \right) = \frac{\partial E}{\partial v_0}(x(x_0, v_0, t), t) \left( \frac{\partial x}{\partial v_0} \right) - \beta \left( \frac{\partial v}{\partial v_0} \right), \quad \frac{\partial v}{\partial v_0}(0) = 1. \] (5.8)

The exact second partial derivatives are solutions to
\[ \frac{d}{dr} \left( \frac{\partial^2 x}{\partial x_0^2 \partial v_0^s} \right) = \frac{\partial^2 v}{\partial x_0^2 \partial v_0^s}, \quad \frac{\partial^2 x}{\partial x_0^2 \partial v_0^s}(0) = 0, \] (5.9)

\[ \frac{d}{dr} \left( \frac{\partial^2 v}{\partial x_0^r \partial v_0^s} \right) = \frac{\partial E}{\partial x_0} \left( \frac{\partial^2 x}{\partial x_0^r \partial v_0^s} \right) - \beta \left( \frac{\partial^2 v}{\partial x_0^r \partial v_0^s} \right) + \frac{\partial^2 E}{\partial x_0^2} \left( \frac{\partial x}{\partial x_0} \right)^r \left( \frac{\partial x}{\partial v_0} \right)^s, \]
\[ \frac{\partial^2 v}{\partial x_0^r \partial v_0^s}(0) = 0, \quad r, s = 0, 1, 2, \quad r + s = 2. \] (5.10)

The approximations to the first and second partial derivatives are obtained by differentiating (5.1), (5.2) with respect to \( x_0, v_0 \). The equations for approximating first partial derivatives with respect to \( x_0 \) are
\[ \frac{d}{dr} \left( \frac{\partial \mathbf{x}}{\partial x_0} \right) = \frac{\partial \mathbf{v}}{\partial x_0}, \] (5.11)

\[ \frac{d}{dr} \left( \frac{\partial \mathbf{v}}{\partial x_0} \right) = \frac{\partial E}{\partial x_0}(\mathbf{x}(t_n), t_n) \frac{\partial \mathbf{x}}{\partial x_0}(t_n) - \beta \left( \frac{\partial \mathbf{v}}{\partial x_0} \right). \] (5.12)
By solving (5.11), (5.12) for \( t_n \leq t \leq t_{n+1} \) and similarly for derivatives with respect to \( v_0 \) the approximate first partial derivatives are obtained as follows: let \( (\partial \chi/\partial x_0)(x_0, v_0, 0) = 1, (\partial \chi/\partial x_0)(x_0, v_0, 0) = 0, (\partial \chi/\partial v)(x_0, v_0, 0) = 0, (\partial \chi/\partial v)(x_0, v_0, 0) = 1 \). Then given \( (\partial \chi/\partial x_0)(x_0, v_0, t_n), (\partial \chi/\partial v)(x_0, v_0, t_n) \) the quantities at time \( t_{n+1} \) are computed as

\[
\frac{\partial \chi}{\partial x_0}(t_{n+1}) = \frac{\partial \chi}{\partial x_0}(t_n) + \left( 1 - e^{-\beta \Delta t} \right) \frac{\partial \chi}{\partial x_0}(t_n) + \left( \frac{\Delta t}{\beta} - \frac{1 - e^{-\beta \Delta t}}{\beta^2} \right) \frac{\partial E}{\partial x}(x(x_0, v_0, t_n), t_n) \frac{\partial \chi}{\partial x_0}(t_n),
\]

(5.13)

\[
\frac{\partial \chi}{\partial v}(t_{n+1}) = e^{-\beta \Delta t} \frac{\partial \chi}{\partial x_0}(t_n) + \left( 1 - e^{-\beta \Delta t} \right) \frac{\partial E}{\partial x}(x(x_0, v_0, t_n), t_n) \frac{\partial \chi}{\partial x_0}(t_n),
\]

(5.14)

\[
\frac{\partial \chi}{\partial v_0}(t_{n+1}) = \frac{\partial \chi}{\partial v_0}(t_n) + \left( 1 - e^{-\beta \Delta t} \right) \frac{\partial \chi}{\partial x_0}(t_n) + \left( \frac{\Delta t}{\beta} - \frac{1 - e^{-\beta \Delta t}}{\beta^2} \right) \frac{\partial E}{\partial x}(x(x_0, v_0, t_n), t_n) \frac{\partial \chi}{\partial x_0}(t_n),
\]

(5.15)

\[
\frac{\partial \chi}{\partial v_0}(t_{n+1}) = e^{-\beta \Delta t} \frac{\partial \chi}{\partial v_0}(t_n) + \left( 1 - e^{-\beta \Delta t} \right) \frac{\partial E}{\partial x}(x(x_0, v_0, t_n), t_n) \frac{\partial \chi}{\partial x_0}(t_n).
\]

(5.16)

The approximate second partial derivatives are obtained as solutions for \( t_n \leq t \leq t_{n+1} \) to

\[
\frac{d}{dt} \left( \frac{\partial^2 \chi}{\partial x_0^2} \right) = \frac{\partial^2 \chi}{\partial x_0^2},
\]

(5.17)

\[
\frac{d}{dt} \left( \frac{\partial^2 \chi}{\partial x_0^2} \right) = \frac{\partial E}{\partial x}(x(t_n), t_n) \left( \frac{\partial^2 \chi}{\partial x_0^2} \right) (t_n) - \beta \left( \frac{\partial^2 \chi}{\partial x_0^2} \right) - \frac{\partial^2 E}{\partial x^2}(x(t_n), t_n) \left( \frac{\partial \chi}{\partial x_0} \right)^r \left( \frac{\partial \chi}{\partial v_0} \right)^s (t_n), \quad r, s = 0, 1, 2, \ r + s = 2.
\]

(5.18)

Thus let \( (\partial^2 \chi/\partial x_0^2)(x_0, v_0)(0) = 0, (\partial^2 \chi/\partial x_0^2)(x_0, v_0)(0) = 0 \) and given quantities at time \( t_n \) then

\[
\frac{\partial^2 \chi}{\partial x_0^2}(t_{n+1}) = \frac{\partial^2 \chi}{\partial x_0^2}(t_n) + \left( 1 - e^{-\beta \Delta t} \right) \frac{\partial^2 \chi}{\partial x_0^2}(t_n) + \left( \frac{\Delta t}{\beta} - \frac{1 - e^{-\beta \Delta t}}{\beta^2} \right) \frac{\partial E}{\partial x}(x(t_n), t_n) \frac{\partial^2 \chi}{\partial x_0^2}(t_n) + \left( \frac{\Delta t}{\beta} - \frac{1 - e^{-\beta \Delta t}}{\beta^2} \right) \frac{\partial^2 E}{\partial x^2}(x(t_n), t_n) \left( \frac{\partial \chi}{\partial x_0} \right)^r \left( \frac{\partial \chi}{\partial v_0} \right)^s (t_n),
\]

(5.19)

\[
\frac{\partial^2 \chi}{\partial x_0^2}(t_{n+1}) = e^{-\beta \Delta t} \frac{\partial^2 \chi}{\partial x_0^2}(t_n) + \left( 1 - e^{-\beta \Delta t} \right) \frac{\partial E}{\partial x}(x(t_n), t_n) \frac{\partial^2 \chi}{\partial x_0^2}(t_n) + \left( 1 - e^{-\beta \Delta t} \right) \frac{\partial^2 E}{\partial x^2}(x(t_n), t_n) \left( \frac{\partial \chi}{\partial x_0} \right)^r \left( \frac{\partial \chi}{\partial v_0} \right)^s (t_n), \quad r, s = 0, 1, 2, \ r + s = 2.
\]

(5.20)

The exact coefficients used in the finite difference equation (4.3) are given by expressions (2.8), (2.9). For the approximate coefficients it will be necessary to require that they are zero for \( x_0, v_0 \) sufficiently large. For this the function \( \chi(x_0, v_0) \in C_0^\infty(R_2) \) is defined so that

\[
\chi(x_0, v_0) = \begin{cases} 
1, & |x_0| + |v_0| \leq R_0 - 1, \\
0, & |x_0| + |v_0| > R_0.
\end{cases}
\]

(5.21)
The approximate coefficients at time \(t_n\) are then given as

\[
\begin{align*}
\overline{a}(x_0, v_0, t_n) &= \chi(x_0, v_0) \exp(\beta t_n) \frac{\partial \chi}{\partial v_0} (x_0, v_0, t_n), \\
\overline{b}(x_0, v_0, t_n) &= \chi(x_0, v_0) \exp(\beta t_n) \frac{\partial \chi}{\partial x_0} (x_0, v_0, t_n), \\
\overline{c}(x_0, v_0, t_n) &= (\chi(x_0, v_0))^2 \exp(3 \beta t_n) \left( \frac{\partial \chi}{\partial v_0} \overline{P}_1 - \frac{\partial \chi}{\partial x_0} \overline{P}_2 \right) (x_0, v_0, t_n), \\
\overline{d}(x_0, v_0, t_n) &= (\chi(x_0, v_0))^2 \exp(3 \beta t_n) \left( \frac{\partial \chi}{\partial x_0} \overline{P}_2 - \frac{\partial \chi}{\partial v_0} \overline{P}_1 \right) (x_0, v_0, t_n).
\end{align*}
\]

Here \(\overline{P}_1, \overline{P}_2\) are the expressions (2.10), (2.11) with the exact partial derivatives replaced with the approximate partial derivatives computed according to (5.13)–(5.16), (5.19), (5.20).

We consider the fully implicit difference method with the exact coefficients of (4.3) replaced with approximate coefficients. Let \(\overline{a}_{i,j}(t_n) = \overline{a}(x_0, v_0, t_n)\) and similarly for \(\overline{b}_{i,j}(t_n), \ldots, \overline{d}_{i,j}(t_n)\). The fully implicit difference method with approximate coefficients is

\[
D_t g_{i,j}^n = q[(\overline{a}_{i,j}(t_{n+1}))^2 D_x^2 g_{i,j}^{n+1} - 2 \overline{a}_{i,j}(t_{n+1}) D_{0,x} D_{0,v} g_{i,j}^{n+1} + (\overline{b}_{i,j}(t_{n+1}))^2 D_v^2 g_{i,j}^{n+1} + \overline{c}_{i,j}(t_{n+1}) D_{0,x} \delta_{i,j}^{n+1} + \overline{d}_{i,j}(t_{n+1}) D_{0,v} \delta_{i,j}^{n+1}]
\]

(5.22)

the goal is to prove that the solutions to (5.22), \(g_{i,j}^n\), converge to \(g(x_0, v_0, t)\), the solution to (2.7), as \(R_0 \to \infty\) and \(\Delta x, \Delta v, \Delta t \to 0\).

To comment on notation in the proofs that follow a generic constant, \(C\), may change value from one expression to the next. Also, the functional dependence of the constant on other quantities may be made explicit or not as needed. We first determine bounds on the solution to (2.3), (2.4) and on their exact and approximate derivatives.

**Lemma 5.1.** Let \(x(x_0, v_0, t), v(x_0, v_0, t)\) be the solution to (2.3), (2.4) such that \(x(x_0, v_0, 0) = x_0, v(x_0, v_0, 0) = v_0\). Assume the constant \(K\) such that \(|E(x, t)| \leq K\). Then if \(|v_0| \leq R_0\) there is a constant \(R = C(R_0)\) that depends on \(R_0\) such that \(|v(x_0, v_0, t)| \leq R\) for \(t > 0\).

**Proof.** Integrating Eq. (2.4) and using the bound \(|E| \leq K\) gives the result

\[
|v(t)| \leq \exp(-\beta t) R_0 + K \left( 1 - \frac{e^{-\beta t}}{\beta} \right) \leq R_0 + \frac{K}{\beta}.
\]

Thus \(C(R_0) = R_0 + K/\beta = R\). \(\square\)

**Lemma 5.2.** Let \(x(x_0, v_0, t), v(x_0, v_0, t)\) be the solution to (2.3), (2.4). For any positive integer \(L\) it is assumed that \(E(x, t)\) and \((\partial^l E/\partial x^l)(x, t)\) are continuous functions for all \(x, t \in [0, T]\) for \(l \leq L\) and that there is a constant \(K\) such that \(|\partial^l E/\partial x^l| \leq K\). Then \((\partial^l/\partial x_0^r \partial v_0^s) x(x_0, v_0, t), (\partial^l/\partial x_0^r \partial v_0^s) v(x_0, v_0, t)\) are continuous functions of \(x_0, v_0, t\), and there are constants \(C_l = C_l(T)\) that depend on \(T\) such that

\[
\begin{align*}
\left| \frac{\partial^l}{\partial x_0^r \partial v_0^s} x(x_0, v_0, t) \right|, & \left| \frac{\partial^l}{\partial x_0^r \partial v_0^s} v(x_0, v_0, t) \right| \leq C_l, \\
0 \leq r, s \leq l, & r + s = l, 1 \leq l \leq L.
\end{align*}
\]

**Proof.** The proof of this lemma is straightforward. First \(l = 1\) is considered. The first partial derivatives with respect to \(x_0\) are solutions to (5.5), (5.6). The existence and uniqueness of the solutions to (5.5), (5.6) continuous in \(t\) and in
the initial values $x_0, v_0$ is guaranteed by standard theory of systems of linear ODEs. Then integrating (5.5), (5.6) and applying the bound on $E$ leads to a Gronwall inequality of the form
\[
\left| \frac{\partial x}{\partial x_0} (t) \right| + \left| \frac{\partial v}{\partial x_0} (t) \right| \leq 1 + K \int_0^t \left( \left| \frac{\partial x}{\partial x_0} (\tau) \right| + \left| \frac{\partial v}{\partial x_0} (\tau) \right| \right) \, d\tau,
\]
with $K = K + 1 + \beta$. Thus
\[
\left| \frac{\partial x}{\partial x_0} (t) \right| + \left| \frac{\partial v}{\partial x_0} (t) \right| \leq \exp(\bar{K} t) \leq \exp(K T) = C_1(T).
\]
The same estimate applies to partial derivatives with respect to $v_0$.

The equations for higher derivatives with respect to $x_0, v_0$ are obtained by differentiating (5.5), (5.6). The equations for $l = 2$ are (5.9), (5.10). The existence and uniqueness of continuous solutions is assumed. Integrating one derives a Gronwall inequality for higher derivatives of the form
\[
\left| \frac{\partial^l x}{\partial x_0^l} v_0^l \right| + \left| \frac{\partial^l v}{\partial x_0^l} v_0^l \right| \leq K \int_0^t \left( \left| \frac{\partial^l x}{\partial x_0^l} v_0^l \right| + \left| \frac{\partial^l v}{\partial x_0^l} v_0^l \right| \right) \, d\tau + K_{l-1}(T) t.
\]
The constant $K_{l-1}(T)$ is a bound on terms involving partial derivatives of $E$ with respect to $x$ and partial derivatives of $x(x_0, v_0, t), v(x_0, v_0, t)$ with respect to $x_0, v_0$ of degree less than $l$. The solution is
\[
\left| \frac{\partial^l x}{\partial x_0^l} v_0^l \right| + \left| \frac{\partial^l v}{\partial x_0^l} v_0^l \right| \leq \left( \frac{e^{\bar{K} t} - 1}{\bar{K}} \right) K_{l-1}(T) = C_l(T)
\]
for $0 \leq t \leq T$. 

A result analogous to Lemma 5.2 is now proved for the approximate particle trajectories given by (5.3), (5.4).

**Lemma 5.3.** Let $(\bar{x}(x_0, v_0, t_n), \bar{v}(x_0, v_0, t_n))$ be the solution to (5.1), (5.2) for $0 \leq t_n \leq T$ and assume the constant $K$ such that $|\partial^l E/\partial x^l| \leq K$ for $l \leq L$. Then there are constants $C_l = C_l(T)$ that depend on $T$ such that
\[
\left| \frac{\partial^l \bar{x}}{\partial x_0^l} (x_0, v_0, t_n) \right|, \left| \frac{\partial^l \bar{v}}{\partial x_0^l} (x_0, v_0, t_n) \right| \leq C_l,
\]
$0 \leq r, s \leq l, r + s = l, 1 \leq l \leq L$.

**Proof.** First $l = 1$ is considered. The first partial derivatives with respect to $x_0$ are computed from (5.11), (5.12). One makes use of the bounds
\[
\frac{1 - e^{-\beta \Delta t}}{\beta} \leq C \Delta t, \quad \left| \frac{\Delta t}{\beta} - \frac{1 - e^{-\beta \Delta t}}{\beta^2} \right| \leq C (\Delta t)^2
\]
and assumes $|\partial E/\partial x| \leq K$. Then from (5.13), (5.14) one obtains inequalities
\[
\left| \frac{\partial \bar{x}}{\partial x_0} (t_n) \right| \leq \left| \frac{\partial \bar{x}}{\partial x_0} (t_{n+1}) \right| + C \Delta t \left| \frac{\partial \bar{v}}{\partial x_0} (t_n) \right| + K C (\Delta t)^2 \left| \frac{\partial \bar{x}}{\partial x_0} (t_n) \right|,
\]
\[
\left| \frac{\partial \bar{v}}{\partial x_0} (t_n) \right| \leq e^{-\beta \Delta t} \left| \frac{\partial \bar{v}}{\partial x_0} (t_{n+1}) \right| + K C (\Delta t) \left| \frac{\partial \bar{x}}{\partial x_0} (t_n) \right|
\]
and
\[
\left| \frac{\partial \bar{x}}{\partial x_0} (t_{n+1}) \right| + \left| \frac{\partial \bar{v}}{\partial x_0} (t_{n+1}) \right| \leq \left| \frac{\partial \bar{x}}{\partial x_0} (t_{n+1}) \right| + \left| \frac{\partial \bar{v}}{\partial x_0} (t_n) \right| + (K C \Delta t + K C (\Delta t)^2) \left| \frac{\partial \bar{x}}{\partial x_0} (t_n) \right| + C \Delta t \left| \frac{\partial \bar{v}}{\partial x_0} (t_n) \right|.
\]
Let $K C (1 + \Delta t) + C = \bar{K}$ and $b_1(t_n) = |(\partial \bar{x}/\partial x_0)(t_n)| + |(\partial \bar{v}/\partial x_0)(t_n)|$. The inequality for $b_1(t_n)$ is
\[
b_1(t_{n+1}) \leq b_1(t_n) + \bar{K} \Delta t b_1(t_n) = (1 + \bar{K} \Delta t) b_1(t_n), \quad b_1(0) = 1.
\]
It follows that \( b_1(t_n) \leq (1 + K \Delta t)^n \). Let \( \Delta t = T/N_t \) and \( t_n = n \Delta t, n = 0, \ldots, N_t \). For \( 0 \leq t_n \leq T \) then
\[
 b_1(t_n) \leq \left( 1 + \frac{K}{N_t} T \right)^n \leq \left( 1 + \frac{K}{N_t} T \right)^{N_t} \leq \exp(\overline{K} T).
\]

Thus
\[
 \left| \frac{\partial \overline{x}}{\partial x_0}(t_n) \right|, \left| \frac{\partial \overline{v}}{\partial x_0}(t_n) \right| \leq \exp(\overline{K} T).
\]

The same type of bound is obtained for \( |(\partial \overline{x}/\partial v_0)(t_n)|, |(\partial \overline{v}/\partial v_0)(t_n)| \). Let \( C_1(T) = \exp(\overline{K} T) \). Then
\[
 \left| \frac{\partial \overline{x}}{\partial x_0}(t_n) \right|, \left| \frac{\partial \overline{v}}{\partial x_0}(t_n) \right| \leq C_1(T)
\]
for \( 0 \leq t_n \leq T \).

For \( l \geq 2 \) the equations for the \( l \)th derivatives with respect to \( x_0, v_0 \) take the form
\[
 \frac{\partial^l \overline{x}}{\partial x_0^l \partial v_0^r}(t_{n+1}) = \frac{\partial^l \overline{x}}{\partial x_0^l \partial v_0^r}(t_n) + \frac{1 - e^{-\beta \Delta t}}{\beta} \frac{\partial^l \overline{v}}{\partial x_0^l \partial v_0^r}(t_n) + \left( \frac{\Delta t}{\beta} - \frac{1 - e^{-\beta \Delta t}}{\beta^2} \right) \frac{\partial E}{\partial x}(\overline{x}(t_n), t_n) \frac{\partial^l \overline{x}}{\partial x_0^l \partial v_0^r}(t_n)
\]
\[
 \quad + \left( \frac{\Delta t}{\beta} - \frac{1 - e^{-\beta \Delta t}}{\beta^2} \right) p(x_0, v_0, t_n),
\]
\[
 \frac{\partial^l \overline{v}}{\partial x_0^l \partial v_0^r}(t_{n+1}) = e^{-\beta \Delta t} \frac{\partial^l \overline{v}}{\partial x_0^l \partial v_0^r}(t_n) + \frac{1 - e^{-\beta \Delta t}}{\beta} \frac{\partial E}{\partial x}(\overline{x}(t_n), t_n) \frac{\partial^l \overline{x}}{\partial x_0^l \partial v_0^r}(t_n)
\]
\[
 \quad + \frac{1 - e^{-\beta \Delta t}}{\beta} p(x_0, v_0, t_n), \quad 0 \leq r, s \leq l, \quad r + s = l.
\]

Here \( p(x_0, v_0, t_n) \) is a sum of terms involving \( \partial^k \overline{x}/\partial x_0^k \partial v_0^i, r + s = k \leq l \leq -1 \) and \( \partial^k E/\partial x^k(\overline{x}(x_0, v_0, t_n), t_n) \), \( 2 \leq k \leq l \). For \( l = 2 \) the equations are (5.19), (5.20). Let \( b_1(t_n) = |(\partial^l \overline{x}/\partial x_0^l \partial v_0^r)(t_n)| + |(\partial^l \overline{v}/\partial x_0^l \partial v_0^r)(t_n)| \). From (5.25), (5.26) one derives an inequality for \( b_1(t_n) \) of the form
\[
 b_1(t_{n+1}) \leq (1 + \overline{K} \Delta t) b_1(t_n) + K_{l-1} \Delta t.
\]

Here \( K_{l-1} = K_{l-1}(T) \) is a constant depending on \( T \) such that \( (C \Delta t + C)|p(x_0, v_0, t_n)| \leq K_{l-1} \) for \( 0 \leq t_n \leq T \). The constant \( C \) is being defined by (5.23). Since \( b_1(0) = 0 \) then \( b_1(t_1) \leq K_{l-1} \Delta t \) and \( b_1(t_2) \leq (1 + \overline{K} \Delta t)(K_{l-1} \Delta t) + (K_{l-1} \Delta t) \) and
\[
 b_1(t_n) \leq [(1 + \overline{K} \Delta t)^n - 1] K_{l-1} \Delta t.
\]

Thus
\[
 b_1(t_n) \leq (1 + \overline{K} \Delta t)^n (K_{l-1} n \Delta t).
\]

Letting \( \Delta t = T/N_t \) then for \( 0 \leq t_n \leq T \)
\[
 b_1(t_n) \leq K_{l-1} T \left( 1 + \frac{K}{N_t} T \right)^{N_t} = K_{l-1} T \left( 1 + \frac{1}{N_t} \frac{T}{K} \right)^T \leq K_{l-1} T \exp(\overline{K} T).
\]
Let $C_I(T) = K_{I-1} T \exp(K T)$. Then
\[
\begin{vmatrix}
\frac{\partial^2 v}{\partial x_0^2} (t_n)
\end{vmatrix}, \begin{vmatrix}
\frac{\partial^2 v}{\partial x_0 \partial v_0} (t_n)
\end{vmatrix} \leq C_I(T)
\]
for $0 \leq t_n \leq T$, $n \leq N_I$. \(\square\)

We now consider the error obtained by replacing exact particle trajectories as solutions to (2.3), (2.4) with approximate trajectories as solutions to (5.1), (5.2). Let $(x(t), v(t)) = (x_0(t_0, t), v_0(t_0, t))$ be the solution to (2.3), (2.4) such that $x(x_0, v_0, T) = x_0$, $v(x_0, v_0, 0) = v_0$ and $(\overline{x}(t), \overline{v}(t)) = (\overline{x}(x_0, v_0, t), \overline{v}(x_0, v_0, t))$ be the solution to (5.1), (5.2) for $t_n \leq t \leq t_{n+1}$ and such that $\overline{x}(x_0, v_0, 0) = x_0$, $\overline{v}(x_0, v_0, 0) = v_0$. The error in particle trajectories is given by

**Lemma 5.4.** Given the constant $R_0$ such that $|x_0| + |v_0| \leq R_0$ then there is a constant $K$ and a constant $K_1 = K_1(R_0)$ depending on $R_0$ such that
\[
|x(x_0, v_0, t_n) - \overline{x}(x_0, v_0, t_n)| + |v(x_0, v_0, t_n) - \overline{v}(x_0, v_0, t_n)| \leq (K_1 T \exp(K T)) \Delta t
\]
for $0 \leq t_n \leq T$.

**Proof.** Taking the difference between solutions to (2.3), (2.4) and (5.1), (5.2) one obtains the equation for $t_n \leq t \leq t_{n+1}$
\[
\frac{d}{dt} (x(t) - \overline{x}(t)) = (v(t) - \overline{v}(t)),
\]
\[
\frac{d}{dt} (v(t) - \overline{v}(t)) = (E(x(t), t) - E(\overline{x}(t_n), t_n)) - \beta(v(t) - \overline{v}(t)).
\]
Eq. (5.29) is integrated as
\[
(v - \overline{v})(t) = e^{-\beta(t-t_n)} (v - \overline{v})(t_n) + \int_{t_n}^{t} e^{\beta(t-s)} (E(x(s), s) - E(\overline{x}(t_n), t_n)) ds.
\]
Now
\[
E(x(t), t) - E(\overline{x}(t_n), t_n) = (E(x(t), t) - E(x(t_n), t_n)) + (E(x(t_n), t_n) - E(\overline{x}(t_n), t_n)).
\]
Let
\[
E(x(t), t) - E(x(t_n), t_n) = \frac{d}{dt} E(x(t), t)|_{t=n}(t - t_n)
\]
for $t_n \leq t_0 \leq t$ and
\[
\frac{d}{dt} E(x(t), t) = \frac{\partial E}{\partial x} \frac{dx}{dt} + \frac{\partial E}{\partial t} = \frac{\partial E}{\partial x} v(t) + \frac{\partial E}{\partial t}.
\]
It is assumed that $|\partial E/\partial x|, |\partial E/\partial t| \leq K$. Then for $|x_0| + |v_0| \leq R_0$ by Lemma 5.1 $|v(t)| \leq R_0 + K/\beta = R$. Thus $|dE/dt| \leq KR + K = K_1(R_0)$ and
\[
|E(x(t), t) - E(x(t_n), t_n)| \leq K_1(t - t_n).
\]
Also,
\[
|E(x(t_n), t_n) - E(\overline{x}(t_n), t_n)| = \left| \frac{\partial E}{\partial x} (z, t_n) \right| |x(t_n) - \overline{x}(t_n)| \leq K |x(t_n) - \overline{x}(t_n)|
\]
with $z \in [x(t_n), \overline{x}(t_n)]$. From (5.30) one obtains the inequality
\[
|(v - \overline{v})(t)| = e^{-\beta(t-t_n)} |(v - \overline{v})(t_n)| + \int_{t_n}^{t} e^{\beta(t-s)} (K_1(s - t_n) + K |x(t_n) - \overline{x}(t_n)|) ds.
\]
Let \( e_x(t) = \max_{t_n \leq s \leq t} |x(s) - \overline{x}(s)| \), \( e_v(t) = \max_{t_n \leq s \leq t} |v(s) - \overline{v}(s)| \). One derives the inequality

\[
e_v(t) \leq e_v(t_n) + \int_{t_n}^{t} (K_1(s - t_n) + K e_x(s)) \, ds.
\]

(5.31)

Integrating (5.28) leads to

\[
e_x(t) \leq e_x(t_n) + \int_{t_n}^{t} e_v(s) \, ds.
\]

(5.32)

Adding (5.31), (5.32) one arrives at the inequality

\[
e_x(t) + e_v(t) \leq \int_{t_n}^{t} (K_1(s - t_n) + K (e_x(s) + e_v(s))) \, ds.
\]

(5.33)

Let \( y(t) = e_x(t) + e_v(t) \) and solving (5.33) leads to the inequality for \( t_n \leq t \leq t_{n+1} \)

\[
y(t) \leq e^{K(t-t_n)} y(t_n) + \int_{t_n}^{t} e^{K(t-s)} K_1(s - t_n) \, ds.
\]

One obtains from this the estimate

\[
y(t_{n+1}) \leq e^{K\Delta t} (y(t_n) + K_1(\Delta t)^2).
\]

For \( n = 0 \), i.e., \( t_0 = 0 \), since \( x(0) = \overline{x}(0) = x_0 \) and \( v(0) = \overline{v}(0) = v_0 \) then \( y(0) = 0 \). Thus \( y(t_1) = e^{K\Delta t} K_1(\Delta t)^2 \),

\[
y(t_2) = e^{K\Delta t} (e^{K\Delta t} K_1(\Delta t)^2 + K_1(\Delta t)^2) \leq e^{2K\Delta t} 2K_1(\Delta t)^2,
\]

and by induction \( y(t_n) \leq e^{nK\Delta t} nK_1(\Delta t)^2 \). For \( \Delta t = T/N_t \) then \( n\Delta t \leq T \) for \( 0 \leq n \leq N_t \). Thus

\[
y(t_n) \leq (e^{K_T} K_1 T)\Delta t
\]

for \( 0 \leq n \leq N_t \). This then gives the inequality (5.27) for \( 0 \leq t_n \leq T \). \( \square \)

Given a bound on the error in the approximate trajectories a similar procedure is followed to obtain bounds on the error in approximate first and second partial derivatives. Taking the difference between Eqs. (5.5), (5.6) and (5.11), (5.12) and making use of Lemma 5.4 a Gronwall type inequality is derived for \( t_n \leq t \leq t_{n+1} \) to bound the difference between exact and approximate first partial derivatives with respect to \( x_0 \). The same type of proof applies for partial derivatives with respect to \( v_0 \). Summing over time intervals for \( 0 \leq t_n \leq T \) provides error bounds for approximate first partial derivatives that depend on \( T \). One then derives error bounds for approximate second partial derivatives. Here a Gronwall type inequality for the error for \( t_n \leq t \leq t_{n+1} \) is obtained by considering the difference between Eqs. (5.9), (5.10) and (5.17), (5.18) and making use of Lemma 5.4 and the error bounds for first partial derivatives. A summation provides the error for the time interval \([0, T]\). While containing some additional technical details the derivation of error bounds for approximate partial derivatives is sufficiently similar to the proof of Lemma 5.4 that we state the following lemma without further proof.

**Lemma 5.5.** Given the constant \( R_0 \) such that \(|x_0| + |v_0| \leq R_0 \) then there are constants \( K \) and \( C = C(R_0, T) \) such that for \( r, s \) nonnegative integers and \( 0 \leq t_n \leq T \)

\[
\left| \frac{\partial^k x}{\partial x_0^r \partial v_0^s}(t_n) - \frac{\partial^k \overline{x}}{\partial x_0^r \partial v_0^s}(t_n) \right| + \left| \frac{\partial^k v}{\partial x_0^r \partial v_0^s}(t_n) - \frac{\partial^k \overline{v}}{\partial x_0^r \partial v_0^s}(t_n) \right| \leq (CTe^{K_T})\Delta t, \quad 0 \leq r, \quad s \leq k, \quad r + s = k, \quad k = 1, 2.
\]

(5.34)
We proceed with a proof that the solution to (5.22) converges to the solution of (2.7). Given the function \( \chi(x_0, v_0) \) defined by (5.21) let

\[
\begin{align*}
\tilde{a}(x_0, v_0, t) &= \chi(x_0, v_0)a(x_0, v_0, t), \\
\tilde{b}(x_0, v_0, t) &= \chi(x_0, v_0)b(x_0, v_0, t), \\
\tilde{c}(x_0, v_0, t) &= (\chi(x_0, v_0))^2c(x_0, v_0, t), \\
\tilde{d}(x_0, v_0, t) &= (\chi(x_0, v_0))^2d(x_0, v_0, t).
\end{align*}
\]

The following lemma gives the error in the coefficients of (5.22).

**Lemma 5.6.** There is a constant \( C = C(R_0, T) \) such that for \( 0 \leq t_n \leq T \) then

\[
|\tilde{a}(x_0, v_0, t_n) - (\tilde{a}(x_0, v_0, t_n))| \leq C \Delta t,
\]

\[
|\tilde{b}(x_0, v_0, t_n) - \chi(x_0, v_0, t_n)| \leq C \Delta t,
\]

\[
|\tilde{c}(x_0, v_0, t_n) - \chi(x_0, v_0, t_n)| \leq C \Delta t,
\]

\[
|\tilde{d}(x_0, v_0, t_n) - \chi(x_0, v_0, t_n)| \leq C \Delta t.
\]

**Proof.** The result follows from the bounds of Lemmas 5.2 and 5.3 and the error in approximate partial derivatives of Lemma 5.5. For example for \( |x_0| + |v_0| \leq R_0 \) then

\[
|\tilde{a}(x_0, v_0, t_n)| = |\tilde{a}(x_0, v_0, t_n) - \chi(x_0, v_0, t_n)| = |\tilde{a}(x_0, v_0, t_n) - \chi(x_0, v_0, t_n)| \leq C(R_0, T) \Delta t.
\]

Similarly for the error in \( (\tilde{b}(x_0, v_0, t_n))^2 \). The error in \( \tilde{a}(x_0, v_0, t) \tilde{b}(x_0, v_0, t), \tilde{c}(x_0, v_0, t), \tilde{d}(x_0, v_0, t) \) involves more complicated algebra but the idea is the same. \( \square \)

Let \( \tilde{a}_{i,j}(t_n) = \tilde{a}(x_0, v_0, t_n) \) and similarly for \( \tilde{b}_{i,j}(t_n), \ldots, \tilde{d}_{i,j}(t_n) \). We define

\[
\bar{L}(g(x_0, v_0, t_n)) = D_{t}g(x_0, v_0, t_n) - q(\bar{a}_{i,j}(t_{n+1}))^2D_x^2g(x_0, v_0, t_{n+1})
\]

\[
- 2\bar{a}_{i,j}D_{0_x}D_{0_v}g(x_0, v_0, t_{n+1}) + \bar{b}_{i,j}(t_{n+1})^2D_x^2g(x_0, v_0, t_{n+1})
\]

\[
+ \bar{c}_{i,j}(t_{n+1})D_{0_x}D_{0_v}g(x_0, v_0, t_{n+1}) + \bar{d}_{i,j}(t_{n+1})D_{0_v}g(x_0, v_0, t_{n+1})
\]

and

\[
R(g(x_0, v_0, t_n)) = (1 - \chi(x_0, v_0, t_n))q(\bar{a}_{i,j}(t_{n+1}))^2D_x^2g(x_0, v_0, t_{n+1})
\]

\[
- 2\bar{a}_{i,j}D_{0_x}D_{0_v}g(x_0, v_0, t_{n+1}) + \bar{b}_{i,j}(t_{n+1})^2D_x^2g(x_0, v_0, t_{n+1})
\]

\[
+ \bar{c}_{i,j}(t_{n+1})D_{0_x}D_{0_v}g(x_0, v_0, t_{n+1}) + \bar{d}_{i,j}(t_{n+1})D_{0_v}g(x_0, v_0, t_{n+1})
\]

Then with the operator \( L(g(x_0, v_0, t_n)) \) defined by (4.13) and by the result of Proposition 4.1 (pointwise consistency)

\[
L(g(x_0, v_0, t_n)) = \bar{L}(g(x_0, v_0, t_n)) - R(g(x_0, v_0, t_n)) = \tau(x_0, v_0, t_n)
\]

with \( \tau(x_0, v_0, t_n) \) given by (4.14). Thus,

\[
\bar{L}(g(x_0, v_0, t_n)) = \tau(x_0, v_0, t_n) + R(g(x_0, v_0, t_n)).
\]

Our assumption is that the solution to (2.7), \( g(x_0, v_0, t) \), as well as partial derivatives of \( g \) of sufficiently high order are continuous, bounded functions and are bounded functions in \( L_2(R_2) \) for each \( t \in [0, T] \). Also, on the basis of
Lemma 5.2 it is determined that \( a_{i,j}(t_n), \ldots, d_{i,j}(t_n) \) are uniformly bounded functions for all \( i, j \) and \( t_n \in [0, T] \). As a result it is assumed that given any \( \varepsilon > 0 \) for \( R_0 \) in (5.21) sufficiently large then

\[
\|R(g)\| = \left( \sum_{i,j} |R(g(x_0, v_0, t_n))|^2 \Delta x \Delta v \right)^{1/2} < \varepsilon
\]

for \( 0 \leq t_n \leq T \), and it is assumed that this holds uniformly in \( \Delta x, \Delta v \) with \( |\Delta x| + |\Delta v| \leq h_0 \) (a small parameter).

For \( g^n_{i,j} \) the solution to (5.22) let

\[
\bar{L}(g^n_{i,j}) = D_t g^n_{i,j} - q[(\alpha_{i,j} + (t_n+1))^2 D^2 g^n_{i,j} + 2\beta_{i,j} D_0 x g^n_{i,j} + (\beta_{i,j} - \bar{b}_{i,j}) (t_n+1) + \bar{c}_{i,j} (t_n+1) + \bar{d}_{i,j} (t_n+1)]
\]

so that \( \bar{L}(g^n_{i,j}) = 0 \). Also, let \( e^n_{i,j} = g(x_0, v_0, t_n) - g^n_{i,j} \) and define

\[
S(g(x_0, v_0, t_n)) = q[(\alpha_{i,j} - \bar{\alpha}_{i,j}) (t_n+1)] D^2 g(x_0, v_0, t_n) + 2(\beta_{i,j} - \bar{b}_{i,j}) (t_n+1) D_0 x g(x_0, v_0, t_n) + (\beta_{i,j} - \bar{b}_{i,j}) (t_n+1) D^2 g(x_0, v_0, t_n) + (\bar{c}_{i,j} - \bar{d}_{i,j}) (t_n+1) D_0 v g(x_0, v_0, t_n) + (\bar{d}_{i,j} - \bar{d}_{i,j}) (t_n+1) D_0 v g(x_0, v_0, t_n)]
\]

Then it can be verified that \( \bar{L}(g(x_0, v_0, t_n)) - \bar{L}(g^n_{i,j}) = S(g(x_0, v_0, t_n)). \) Combined with (5.36) it follows that \( \bar{L}(e^n_{i,j}) - S(g(x_0, v_0, t_n)) = \tau(x_0, v_0, t_n) + R(g(x_0, v_0, t_n)). \) Thus,

\[
\bar{L}(e^n_{i,j}) = \tau(x_0, v_0, t_n) + R(g(x_0, v_0, t_n)) + S(g(x_0, v_0, t_n)).
\]

The proof of convergence of the solution to (5.22) involves showing that \( ||e^n|| = (\sum_{i,j} |e^n_{i,j}|^2 \Delta x \Delta v)^{1/2} \to 0 \) as \( \Delta x, \Delta v, \Delta t \to 0 \). This result is stated as

**Theorem 5.1.** Given any \( \varepsilon > 0 \) and time \( T \) then there exists a \( \delta > 0 \) such that \( ||e^n|| < \varepsilon \) for \( 0 \leq t_n \leq T \) whenever \( (\Delta x)^2 + (\Delta v)^2 + \Delta t < \delta \).

**Proof.** Let \( \gamma(x_0, v_0, t_n) = \tau(x_0, v_0, t_n) + R(g(x_0, v_0, t_n)) + S(g(x_0, v_0, t_n)) \) so that \( \bar{L}(e^n_{i,j}) = \gamma(x_0, v_0, t_n) \). For \( \varepsilon_1 \) to be determined it is assumed that in (5.21) \( R_0 = R_0(\varepsilon_1) \) is sufficiently large so that \( ||R(\gamma, t_n)|| < \varepsilon_1 \) for \( 0 \leq t_n \leq T \) and for all \( \Delta x, \Delta v \) with \( \sqrt{(\Delta x)^2 + (\Delta v)^2} \leq h_0 \) (small parameter). By Lemma 5.6 \( |\alpha_{i,j}(t_n) - \bar{\alpha}_{i,j}(t_n)| \leq C(R_0, T) \Delta t \) and similarly for the other differences of coefficients in \( S(g(x_0, v_0, t_n)) \). Thus

\[
||S(g(\gamma, t_n))|| \leq C(R_0, T) \Delta t (||D^2 g|| + ||D_0 x D_0 v g|| + ||D_v^2 g|| + ||D_0 x g|| + ||D_0 v g||) \leq C(R_0, T) \Delta t.
\]

Also, from (4.14)

\[
||\gamma(\gamma, t_n)|| \leq C(T) ||e_1|| (||\Delta x||^2 ||c_2|| + ||\Delta v||^2 ||c_3||) \leq C(T)(\Delta t + (\Delta x)^2 + (\Delta v)^2).
\]

Thus

\[
||\gamma(\gamma, t_n)|| \leq C(T)(\Delta t + (\Delta x)^2 + (\Delta v)^2) + C(R_0(\varepsilon_1), T) \Delta t + \varepsilon_1
\]

\[
= C(T)((\Delta x)^2 + (\Delta v)^2) + C(T) + C(R_0(\varepsilon_1), T) \Delta t + \varepsilon_1
\]

\[
= C(T)((\Delta x)^2 + (\Delta v)^2) + C(R_0(\varepsilon_1), T) \Delta t + \varepsilon_1.
\]

(5.37)
We assume on the basis of Lemma 5.3 that

\[ |D_x^2 a_{i,j}| \leq K_1, \quad |D_v^2 b_{i,j}| \leq K_3, \quad |D_x D_v(2a b_{i,j})| \leq K_2, \]

\[ |D_x D_v(2a b_{i,j})|_{i,j-1} \leq K_2, \quad |D_x \bar{e}_{i,j}| \leq K_4, \quad |D_v \bar{d}_{i,j}| \leq K_5 \]

and \( K = K(T) = K_1 + K_2 + K_3 + K_4 + K_5 \). Then \( \bar{L}(e_{i,j}) = \gamma(x_0, v_0, t_n) \) is written as

\[
e_{i,j}^{n+1} = e_{i,j}^n + (\Delta t)q1(i(a_1, j(t_{n+1}))^2 D_x^2 e_{i,j}^{n+1} - 2a_{i,j}^n(t_{n+1})\bar{e}_{i,j}(t_{n+1})D_0 e_{i,j}^{n+1} + (\bar{e}_{i,j}(t_{n+1}))^2 D_v e_{i,j}^{n+1}
\]

\[ + \bar{e}_{i,j}(t_{n+1})D_0 e_{i,j}^{n+1} + \bar{d}_{i,j}(t_{n+1})D_v e_{i,j}^{n+1} + \Delta t \gamma(x_i, v, t_n). \]

As in the proof of Theorem 4.2 one derives the inequality

\[
\|e^{n+1}\|^2 \leq \|e^n\|^2 + \Delta t K \|e^{n+1}\|^2 + 2\Delta t \|e^{n+1}\|\|\gamma(\cdot, t_n)\|.
\]

This inequality is the same form as (4.17). With (5.37) the inequality is

\[
\|e^{n+1}\|^2 \leq \|e^n\|^2 + \Delta t K \|e^{n+1}\|^2 + 2\Delta t \|e^{n+1}\|\|C(T)((\Delta x)^2 + (\Delta v)^2) + C(R_0(e_1), T)\Delta t + e_1\|.
\]

One, therefore, follows similar reasoning continuing from (4.17) in the proof of Theorem 4.2 to derive

\[
\|e^{n+1}\| \leq \frac{\|e^n\|}{\sqrt{1 - K q \Delta t}} + \frac{2\Delta t [C(T)((\Delta x)^2 + (\Delta v)^2) + C(R_0(e_1), T)\Delta t + e_1]}{1 - K q \Delta t}.
\]

Let \( \Delta t = T/N_t \) with \( N_t \) sufficiently large so that \( K q < 1/(2qK) \) and therefore \( \frac{1}{2} < 1 - K q \Delta t < 1 \). It follows that

\[
\|e^n\| \leq \frac{2\sqrt{2}T}{(1 - K q \Delta t)^{n/2}} \frac{C(T)((\Delta x)^2 + (\Delta v)^2) + C(R_0(e_1), T)\Delta t + e_1}{N_t}. \]

For \( 0 \leq n \leq N_t \) then

\[
\|e^n\| \leq \frac{2\sqrt{2}T}{(1 - K q \Delta t)^{n/2}} \frac{C(T)((\Delta x)^2 + (\Delta v)^2) + C(R_0(e_1), T)\Delta t + e_1}{N_t}.
\]

As shown in the proof of Theorem 4.2

\[
\frac{1}{(1 - K q \Delta t)^{n/2}} \leq 2^{K q T}.
\]

Thus

\[
\|e^n\| \leq 2\sqrt{2}T \frac{C(T)((\Delta x)^2 + (\Delta v)^2) + C(R_0(e_1), T)\Delta t + e_1}{N_t} \leq C(T)((\Delta x)^2 + (\Delta v)^2) + C(R_0(e_1), T)\Delta t + C(T)e_1.
\]

(5.38)

Given \( \varepsilon > 0 \) then let \( C(T)e_1 < \varepsilon/3, \) i.e., \( e_1 < \varepsilon/(3C(T)) \). The \( e_1 \) then determines \( R_0 \) of (5.21) and the small parameter \( h_0 \) specified above so that \( \|R(g(\cdot, t_0))\| < e_1 \) for \( \sqrt{(\Delta x)^2 + (\Delta v)^2} \leq h_0. \) Let \( \delta_1 = \min\{e/3C(T), h_0^2\} \) so that \( (\Delta x)^2 + (\Delta v)^2 < \delta_1 \) then \( C(T)((\Delta x)^2 + (\Delta v)^2) < \varepsilon/3. \) Having specified \( e_1 \) and \( R_0 = R_0(e_1) \) then the constant \( C(R_0(e_1), T) \) of (5.38) is determined. Let \( \delta_2 = \min\{e/3C(R_0(e_1), T), 1/2qK\} \) so that for \( \Delta t < \delta_2 \) then \( C(R_0(e_1), T)\Delta t < \varepsilon/3. \) Finally, let \( \delta = \min\{\delta_1, \delta_2\}. \) If \( \Delta t + (\Delta x)^2 + (\Delta v)^2 < \delta \) then from (5.38)

\[
\|e^n\| \leq C(T)\delta_1 + C(R_0(e_1), T)\delta_2 + C(T)e_1 \leq C(T)\frac{\delta_1}{3C(T)} + C(R_0(e_1), T)\frac{\delta_2}{3C(R_0(e_1), T)} + C(T)\frac{\varepsilon}{3C(T)} = \varepsilon.
\]
6. The numerical method

The analysis that is carried out in Sections 3–5 is for a discretization of the initial value problem (2.7) combined with (2.8)–(2.11). This is a simpler and more idealized problem than what is solved computationally. For the computational problem the periodic boundary condition in x is introduced, and the further transformation of velocity space is carried out according to (2.12) to get Eq. (2.13). The numerical method is based on obtaining the solution to (1.1) in terms of a sequence of solutions to (2.13). For the time interval [0, T] then \( T > 0 \) is such that \( T / T_1 = M \) an integer. For \( l = 0, 1 \ldots, M \) let \( \tau_l = lT_1, t \in [0, T_1], \tilde{t} = \tau_l + t \). On the time interval \( \tilde{t} \in [\tau_l, \tau_{l+1}] \) then

\[
f(x, v, \tilde{t}) = e^{\beta \tilde{t}} g(x_0(x, v, t), u(v_0(x, v, t)), t).
\]

Here \( x_0(x, v, t), v_0(x, v, t) \) is the inverse transformation (2.6), \( u(v_0) \) is the inverse of (2.12), and \( g(x_0, u, t) \) is the solution to (2.13) for \( t \in [0, T_1] \) such that \( g(x_0, u, 0) = f(x_0, cu/\sqrt{1 - u^2}, \tau_l) \). If \( l = 0, \tau_l = 0 \) then \( f(x, v, \tau_l) = f_0(x, v) \). If \( l > 0 \) then \( f(x, v, \tau_l) = e^{\beta \tau_l} g(x_0(x, v, T_1), u(v_0(x, v, T_1)), T_1) \) and such that \( g(x_0, u, t) \) is the solution to (2.13) for \( \tilde{t} \in [\tau_{l-1}, \tau_l] \). The numerical method discretizes this process. The method of approximation can be viewed as a type of deterministic particle method in which the solution to (1.1) is computed along particle trajectories approximating the solutions to (2.16), (2.17). The function values along trajectories are obtained from the finite difference approximation of (2.13) which is carried out on a fixed grid. The particle computation is supplemented with a periodic interpolation of the solution along trajectories onto the fixed grid for approximating (2.13). The difference equation for (2.13) is then reinitialized with the interpolated data as the new initial function, and the particle computation is restarted.

A brief description of the numerical approximation is given with details referred to [19]. The computational procedure is based on approximating (2.13) by a semi-implicit difference method as is done in [19]. However, since the analysis of Sections 4 and 5 is for a fully implicit difference method we also include in the description the procedure for computing with a fully implicit difference method. A comparison between the semi-implicit and fully implicit methods for approximating (2.13) is given in Section 7.

6.1. Outline of the numerical method

1. Partition of phase space and time intervals: Let \( \Omega = \{(x_0, u)/0 \leq x_0 \leq L, -1 < u < 1\} \). The partition of \( \Omega \) is given by (3.11) (also by [19, (2.1)]). The points \((x_{0i}, u_{ij})\), \(i = 1, \ldots, N_x, j = 1, \ldots, N_v\) of (3.11) provide the uniform grid for approximating (2.13) by a finite difference method. Let

\[
v_{0ij} = cu_j/\sqrt{1 - u_j^2}. \tag{6.1}
\]

The points \((x_{0i}, v_{0ij})\) are the initial points for particle trajectories approximating the solution to (2.16), (2.17). The total number of particles in phase space is \( N = N_x N_v \).

To discretize the time interval \([0, T]\) let \( T_1 < T \) be such that \( MT_1 = T \) for positive integer \( M \). For positive integer \( N_g \) let \( \Delta t = T_1 / N_g \). The time interval for the particle computation is \([0, T_1]\) and is discretized as \( t_n = n \Delta t, n = 0, 1, \ldots, N_g \). The initializing and regriding of the solution is done at times \( \tau_l = lT_1, l = 0, 1, \ldots, M \). Let \( k = lN_g + n \). The actual time of the computation is \( \tilde{t}_k = \tau_l + t_n, k = 0, 1, \ldots, N_t \) where \( N_t = MN_g \).

2. The deterministic particle method on the time interval \([0, T_1]\):

(i) The approximation of (2.13): Let \( g^n_{i,j} \) be the approximation to \( g(x_0, u_j, t_n) \). If \( l = 0, n = 0 \), i.e., \( k = 0, \tilde{t}_k = 0 \) then let

\[
\tilde{S}_{i,j}^0 = f_0(x_{0i}, v_{0ij}), \quad v_{0ij} = \frac{cu_j}{\sqrt{1 - u_j^2}}, \quad i = 1, \ldots, N_x, \quad j = 1, \ldots, N_v.
\]

It is assumed that

\[
\int_0^L \int_{-\infty}^\infty f_0(x, v) \, dv \, dx = \int_0^L \int_{-1}^1 f_0 \left( x_0, \frac{cu}{\sqrt{1 - u^2}} \right) \frac{c}{(1 - u^2)^{3/2}} \, du \, dx_0 = K.
\]
Thus the computation is initialized at \( t_0 = 0 \) to preserve the \( L_1 \) norm of the initial data. This is equivalent in the context of [19, p. 610] to normalizing the initial data to preserve charge neutrality. If \( l > 0 \), \( n = 0 \), i.e., \( \tilde{t}_k = lT_1 = t_l \) and \( t_n = 0 \), then \( \tilde{q}^{0}_{i,j} \) is obtained from the regridding process addressed in part 3.

At time \( t_n \) we assume approximate coefficients \( a_{i,j}(t_n), d_{i,j}(t_n) \). Then given \( \tilde{g}^{n}_{i,j}, n = 0, 1, \ldots, N_y - 1 \) to get \( g^{n+1}_{i,j} \) we compute \( \tilde{g}^{n+1}_{i,j} \) as the solution to the semi-implicit difference equation (the notation is according to (3.2), (3.13), (3.14))

\[
\tilde{g}^{n+1}_{i,j} = g^{n}_{i,j} + q\Delta t[(a_{i,j}(t_n))(u^{n}_{i,j}) - 2a_{i,j}(t_n)\partial_x D_{0,x} g^{n}_{i,j} + (b_{i,j}(t_n))\partial_u D_{0,u} g^{n}_{i,j}]
\]

The boundary conditions for (6.2) are the same as for (3.15). The difference equation (6.2) is either solved by the iterative procedure SOR or by the direct Douglas–Rachford method as explained in [19, Section 2.2.2]. We let

\[
\lambda = \frac{1}{K} \left( \sum_{i,j} c \frac{g^{n+1}_{i,j}}{(1-u^2_j)^{3/2}} \Delta u \Delta x \right)
\]

and then \( g^{n+1}_{i,j} = \frac{\tilde{g}^{n+1}_{i,j}}{\lambda} \). Thus the computed solution is normalized at each step of the computation to preserve the \( L_1 \) norm (or total charge). This makes the present computation consistent with the procedure of [19, p. 613] in which the computed solution is normalized at each step to preserve charge neutrality.

(ii) Approximation of (2.16), (2.17), particle trajectories: The approximation to (2.16), (2.17) with initial point \((x_0, v_0)\) at time \( t_0 \) is denoted \( x(i, j, t_0), v(i, j, t_0) \). Thus \( x(i, j, 0) = x_0, v(i, j, 0) = v_0 \), and given \( x(i, j, t_n), v(i, j, t_n) \) the computation of \( x(i, j, t_{n+1}), v(i, j, t_{n+1}) \) proceeds according to the discretization of (2.16), (2.17) given in [19, Section 2.2.3]. However, in the present paper the self-consistent electric field \( \overline{E}(x, t) \) of [19, (2.18), (2.19)] is replaced with the given external field, \( E(x, t) \).

(iii) Approximation of first partial derivatives and coefficients \( a_{i,j}(t_n), b_{i,j}(t_n) \): Approximate first partial derivatives of the \( i, j \)th trajectory with respect to \( x_0, v_0 \) are computed as in [19, Section 2.2.4]. Given partial derivatives at time \( t_n \) then partial derivatives at time \( t_{n+1} \) are computed according to expressions [19, (2.20)–(2.23)] in which \( \partial E/\partial x(x(i, j, t_n), t_n) \) is replaced with \( (\partial \overline{E}/\partial x(x(i, j, t_n), t_n)) \). The coefficients \( a_{i,j}(t_{n+1}), b_{i,j}(t_{n+1}) \) are then given at the end of [19, Section 2.2.4].

(iv) Approximation of second partial derivatives and coefficients \( c_{i,j}(t_n), d_{i,j}(t_n) \): Approximate second partial derivatives of the \( i, j \)th trajectory with respect to \( x_0, v_0 \) are computed as in [19, Section 2.2.5]. Given second partial derivatives at time \( t_n \) then second partial derivatives at time \( t_{n+1} \) are computed according to [19, (2.24), (2.25)] in which derivatives of the exact field \( E(x, t) \) replace derivatives of the self-consistent field. The coefficients \( c_{i,j}(t_{n+1}), d_{i,j}(t_{n+1}) \) are then obtained as in [19, Section 2.2.5].

3. Regriding the solution: As described in [19, Section 2.2.6] the approximate trajectory \( x(i, j, t_n), v(i, j, t_n) \) is considered to be the path of an element of charge in phase space given by

\[
q^n_{i,j} = \frac{cg^n_{i,j}}{(1-u^2_j)^{3/2}} \Delta u \Delta x.
\]

Here \( g^n_{i,j} \) is computed above in part 2(i). At times \( t_l = lT_1, l = 1, 2, \ldots, M \) this solution along particle trajectories computed in part 2 is interpolated onto the fixed grid given by (3.11) as discussed in part 1. The process is described
in detail in [19, Section 2.3]. Thus, when \( n = N_g, t_n = T_1 \) the charge elements \( q_{i,j}^n \) at locations in phase space \((x(i, j, t_n), v(i, j, t_n))\) are used to construct a new initial function \( g_{i,j}^0 \) for (6.2). The particle computation of part 2 is then restarted with \( t_n = 0 \), and the computation of part 2 proceeds for \( \tilde{t}_k \) in the interval \([lT_1, (l + 1)T_1]\).

4. The solution on the time interval \([0, T]\): Quantities that are computed to represent the solution to (1.1) are the kinetic energy and the free energy. For \( \tilde{t} \in [0, T] \) the kinetic energy, \( ke(\tilde{t}) \), is precisely as in [19, Section 2.4]. The discretized version of \( ke(\tilde{t}) \), denoted \( ke(\tilde{t}_k) \), is given by [19, (2.37)] for \( 0 \leq \tilde{t}_k \leq T \). As stated in [3] the free energy is defined by \( FE(\tilde{t}) = ke(\tilde{t}) + pe(\tilde{t}) - q/\beta \text{ent}(\tilde{t}) \) where \( pe(\tilde{t}) \) is the potential energy associated with Eq. (1.1) and \( \text{ent}(\tilde{t}) \) is the entropy. The entropy is defined as in [19, Section 2.4]. The discrete version, \( \text{ent}(\tilde{t}_k) \), is computed according to [19, (2.38)]. The potential energy is defined by

\[
pe(\tilde{t}) = \int_0^L \int_{-\infty}^{\infty} \phi_0(x, \tilde{t}) f(x, v, \tilde{t}) \, dv \, dx
\]

in which \( \phi_0(x, \tilde{t}) \) is the electric potential such that \( E(x, \tilde{t}) = -\tilde{\phi}(x, \tilde{t}) \). For this periodic problem an arbitrary constant of integration in the function \( \phi_0(x, \tilde{t}) \) is chosen so that \( \phi_0(0, \tilde{t}) = \phi_0(L, \tilde{t}) = 0 \). For \( \tilde{t} \in [lT_1, (l + 1)T_1] \) and \( t = \tilde{t} - lT_1 \) then in terms of the solution to (2.13), (2.16), (2.17)

\[
\begin{align*}
pe(\tilde{t}_k) &= \sum_{i,j} \phi_0(x(i,j,\tilde{t}_k), \tilde{t}_k) g_{i,j}^n \frac{c}{(1 - u_j^2)^{3/2}} \Delta u \Delta x. \\
\end{align*}
\]

Thus from (6.4) and [19, (2.37), (2.38)] the free energy is then approximated as \( FE(\tilde{t}_k) = ke(\tilde{t}_k) + pe(\tilde{t}_k) - q/\beta \text{ent}(\tilde{t}_k) \).

A summary of the numerical method is given in [19, Section 2.4.1]. To apply this summary to the present paper the following changes are made: the approximations to the trajectory and equations for the first and second partial derivatives discussed in Section 6.1, part 2(ii)–(iv) use the known electric field, \( E(x, t) \), and not the self-consistent electric field, \( \overline{E}(x, t) \). The computation of free energy as given by expression [3, (1.12), (1.13)] involves only the known external potential and not an internally consistent electric field. The computation of an electric field by the particle-in-cell method, which is part of the computation in [19], is not included in the numerical procedure of the present paper. With these changes the summary of the numerical method given in [19] can be followed for the computations in the present paper.

**6.2. Computation of the fully implicit difference method**

An analysis of the stability and convergence of the fully implicit difference method as an approximation to the initial value problem (2.7) is carried out in Sections 4 and 5. For the purpose of actual computation this method is adapted to the initial, boundary value problem (2.13). This is done by modifying the algorithm for computing the semi-implicit difference method described in Section 6.1, part 2(i) to apply to the fully implicit difference method. Eq. (6.2) is replaced with

\[
\begin{align*}
g_{i,j}^{n+1} &= g_{i,j}^n + q \Delta t [(a_{i,j}(t_n+1))^2 D_{x_{i,j}}^2 g_{i,j}^{n+1} - 2a_{i,j}(t_n+1)b_{i,j}(t_n+1)D_{x_{i,j}} D_{u_{i,j}} g_{i,j}^{n+1} + (b_{i,j}(t_n+1))^2 D_{u_{i,j}}^2 g_{i,j}^{n+1} \\
&+ c_{i,j}(t_n+1)D_{x_{i,j}} D_{u_{i,j}} g_{i,j}^{n+1} + d_{i,j}(t_n+1)D_{u_{i,j}} g_{i,j}^{n+1}],
\end{align*}
\]

If \( i = 1 \) then \( g_{i-1,j}^{n+1} = g_{N_x,j}^{n+1} \), if \( i = N_x \) then \( g_{i+1,j}^{n+1} = g_{1,j}^{n+1} \). If \( j = 1 \) then \( g_{i,j-1}^{n+1} = 0 \) and if \( j = N_v \) then \( g_{i,j+1}^{n+1} = 0 \).

The solution to (6.5) is obtained by an iterative procedure based on the equation

\[
\begin{align*}
g_{i,j}^{l+1} &= g_{i,j}^n + q \Delta t [(a_{i,j}(t_n))^2 D_{x_{i,j}}^2 g_{i,j}^{l+1} - 2a_{i,j}(t_n)b_{i,j}(t_n+1)D_{x_{i,j}} D_{u_{i,j}} g_{i,j}^{l+1} + (b_{i,j}(t_n))^2 D_{u_{i,j}}^2 g_{i,j}^{l+1} \\
&+ c_{i,j}(t_n)D_{x_{i,j}} D_{u_{i,j}} g_{i,j}^{l+1} + d_{i,j}(t_n)D_{u_{i,j}} g_{i,j}^{l+1}],
\end{align*}
\]

with \( l = 0, 1, 2, \ldots \). Eq. (6.6) is a semi-implicit equation in the index of iteration \( l \) in which \( g_{i,j}^n \) is a fixed quantity. Thus, given \( g_{i,j}^n \) to get \( g_{i,j}^{n+1} \) let \( g_{i,j}^0 = g_{i,j}^n \) and given \( g_{i,j}^l \) one obtains \( g_{i,j}^{l+1} \) by solving the semi-implicit equation (6.6).
using either the SOR or Douglas–Rachford method described in [19, Section 2.2.2]. Then \( l + 1 \rightarrow l \), \( \tilde{g}_{i,j}^{l+1} \rightarrow \tilde{g}_{i,j}^{l} \), and the solution to (6.6) is repeated. This iterative procedure continuous until \( \max_{i,j} |\tilde{g}_{i,j}^{l+1} - \tilde{g}_{i,j}^{l}| \) is sufficiently small.

Then \( \tilde{g}_{i,j}^{n+1} = \tilde{g}_{i,j}^{l+1} \), and \( \tilde{g}_{i,j}^{n+1} \) is taken to be the solution to (6.5). For \( K \) given in Section 6.1, part 2(i) let

\[
\lambda = \frac{1}{K} \left( \sum_{i,j} \tilde{g}_{i,j}^{n+1} \frac{c}{(1 - u_j^2)^{3/2} \Delta u \Delta x} \right)
\]

and \( \tilde{g}_{i,j}^{n+1} = \tilde{g}_{i,j}^{n+1} / \lambda \). To compute the solution to (1.1) based on the fully implicit difference method this iterative procedure based on Eq. (6.6) replaces the procedure for solving the semi-implicit equation (6.2) in Section 6.1, part 2(i).

To incorporate the fully implicit difference method (6.5) into the overall numerical approximation some changes are made to the summary of operations given in [19, Section 2.4.1]. Since the coefficients in (6.5) are evaluated at time \( t_{n+1} \) these coefficients need to be computed before applying the iterative procedure (6.6). The steps of the particle computation are listed in the summary under part (3). To compute with the fully implicit method (6.6) these steps should be in the order: given quantities at time \( t_n \) to get updated quantities at \( t_{n+1} \)

(i) compute approximate second partial derivatives;
(ii) compute approximate first partial derivatives;
(iii) obtain coefficients \( a_{i,j}(t_{n+1}), b_{i,j}(t_{n+1}), c_{i,j}(t_{n+1}), d_{i,j}(t_{n+1}) \);
(iv) compute \( \tilde{g}_{i,j}^{n+1} \) based on (6.6);
(v) compute particle trajectories \( x(i, j, t_{n+1}), v(i, j, t_{n+1}) \).

We do not provide a proof of the convergence of the algorithm (6.6) for solving the fully implicit difference method; however, in all computations done the algorithm based either on SOR or Douglas–Rachford converged with a relatively small number of iterations in the index \( l \). Also, the primary purpose for computing the fully implicit difference method is to establish a correspondence between the analysis of stability and convergence that is given in Sections 4 and 5 and actual computation.

7. Computational examples

7.1. Numerical verification of convergence

If the function, \( E(x, t) \), in (1.1) is a function only of \( x \), i.e., \( E(x, t) = E(x) \) and \( E(x) = -\partial \phi_0 / \partial x \) for the potential function \( \phi_0(x) \), then the steady state solution to (1.1) is

\[
f_s(x, v) = \frac{K}{C \sqrt{2\pi(q/\beta)}} \exp \left( -\frac{v^2}{2} + \frac{\phi_0(x)}{q/\beta} \right),
\]

where

\[
K = \int_0^L \int_{-\infty}^{\infty} f_0(x, v) \, dv \, dx
\]

and

\[
C = \int_0^L \exp \left( -\frac{\phi_0(x)}{q/\beta} \right) \, dx.
\]

The form of the steady state is given in [3, Theorem A, p. 491] for an initial value problem in three dimensions. However, we can assume for the potential \( \phi_0(x) \) that \( \phi_0(0) = \phi_0(L) = 0 \), and the form of [3, Theorem A] is then adapted to the present 1-D periodic problem as given by (7.1).
The steady state solution (7.1) then gives us an exact solution to (1.1) that we can use to test the convergence and accuracy of the computed solution to (1.1). The error in the computed solution is measured in terms of a discrete \( L_2 \) norm which is defined in the following way. We assume the time interval \([0, T]\) to be subdivided as described at the beginning of Section 6 into subintervals \([\tau_l, \tau_{l+1}]\), \(\tau_l = lT_1\), \(l = 0, 1, \ldots, M\). Then let \(\tilde{t} \in [\tau_l, \tau_{l+1}]\), \(\tilde{t} = \tau_l + \Delta t\). The \( L_2 \) norm of \( f(x, v, \tilde{t}) \) is

\[
\| f(\cdot, \tilde{t}) \|_2 = \left( \int_0^L \int_{-\infty}^\infty (f(x, v, \tilde{t}))^2 \, dv \, dx \right)^{1/2}.
\]

Based on the transformations of independent variables defined by (2.5) and (2.12) the change of variables in the integral are \((x, v) \rightarrow (x_0, v_0)\) and then \((x_0, v_0) \rightarrow (x_0, u)\). In terms of variables \((x_0, u)\) then the \( L_2 \) norm is written as

\[
\| f(\cdot, \tilde{t}) \|_2 = \left( \int_0^L \int_{-1}^1 (f(x_0, v_0(u), t), v(x_0, v_0(u), t), \tilde{t}))^2 e^{-\beta t} \frac{c}{(1-u_j^2)^{3/2}} \, du \, dx_0 \right)^{1/2}.
\]

For data points \((x_0, v_0)\) where \(v_0 = v_0(u_j) = cu_j/\sqrt{1-u_j^2}\) and discrete time \(t_n = n\Delta t\) and \(\tilde{t}_k = \tau_l + t_n\) then a discrete \( L_2 \) norm, referred to as the \( l_{2,A} \) norm, can be defined as

\[
\| f \|_{2,A} = \left( \sum_{i,j} (f(x_0, v_0(u_j), t_n), v(x_0, v_0(u_j), t_n), \tilde{t}_k))^2 e^{-\beta t_n} \frac{c}{(1-u_j^2)^{3/2}} \Delta u \Delta x \right)^{1/2}.
\]

Here \( f \) is the exact solution to (1.1), and \( x(x_0, v_0(u_j), t_n), v(x_0, v_0(u_j), t_n) \) are the exact solutions to (2.16), (2.17) with initial points \(x_0, v_0(u_j)\) at time \(t_n\). The \( l_{2,A} \) norm is now being defined somewhat differently than in Sections 3–5. Let \(\tilde{f}(x(i, j, t_n), v(i, j, t_n), \tilde{t}_k)\) be the approximation to \(f(x(x_0, v_0(u_j), t_n), v(x_0, v_0(u_j), t_n), \tilde{t}_k)\). Then \((x(i, j, t_n), v(i, j, t_n))\) is the approximate trajectory given in Section 6.1, part 2(ii) and \(\tilde{f}(x(i, j, t_n), v(i, j, t_n), \tilde{t}_k) = e^{\beta t_n} g_{i,j}^n\) such that \(g_{i,j}^n\) is the normalized solution to (6.2) or (6.5) at time \(t_n \in [0, T_1]\) and \(\tilde{t}_k = \tau_l + t_n\). The square of the error in the discrete approximation in the \( l_{2,A} \) norm is defined as

\[
\| f - \tilde{f} \|_{2,A}^2 = \sum_{i,j} (f(x_0, v_0(u_j), t_n), v(x_0, v_0(u_j), t_n), \tilde{t}_k) - \tilde{f}(x(i, j, t_n), v(i, j, t_n), \tilde{t}_k))^2 e^{-\beta t_n} \frac{c}{(1-u_j^2)^{3/2}} \Delta u \Delta x
\]

\[
= \sum_{i,j} (f(x_0, v_0(u_j), t_n), v(x_0, v_0(u_j), t_n), \tilde{t}_k) - e^{\beta t_n} g_{i,j}^n)^2 e^{-\beta t_n} \frac{c}{(1-u_j^2)^{3/2}} \Delta u \Delta x.
\]

Even if we have an exact function, \( f \), for the solution to (1.1) in general we do not have expressions for the exact trajectories \(x(x_0, v_0(u_j), t_n), v(x_0, v_0(u_j), t_n)\) for \(t_n > 0\). Thus for \(t_n > 0\) we cannot precisely measure the discrete \( L_2 \) error even with a known solution. However, at \(t_n = 0, \tilde{t}_k = \tau_l\) then \(x(x_0, v_0(u_j), 0) = x_0, v(x_0, v_0(u_j), 0) = v_0 = cu_j/(1-u_j^2)^{3/2}\). Then

\[
\| f - \tilde{f} \|_{2,A}^2 = \sum_{i,j} (f(x_0, v_0(u_j), \tau_l) - g_{i,j}^0)^2 \frac{c}{(1-u_j^2)^{3/2}} \Delta u \Delta x.
\]

In this expression \( f(x_0, v_0(u_j), \tau_l) = f(x_0, cu_j/\sqrt{1-u_j^2}, \tau_l) \) is exactly evaluated if \( f \) is a known function and \(g_{i,j}^0\) is the initial function for (6.2) or (6.5) at \(\tilde{t}_k = \tau_l, t_n = 0\). As discussed in Section 6.1, part 2(i) if \(l = 0\) then \(g_{i,j}^0\) is obtained from the initial function for (1.1), \(f_0(x, v)\). If \(l > 0\) then \(g_{i,j}^0\) is obtained from the regridding, Section 6.1, part 3. Therefore the error of the numerical method is computed at times \(\tau_l, l = 0, 1, \ldots, M\) and will be given as a relative discrete \( L_2 \) error. Let \(f_\epsilon(x, v, \tau_l)\) be the exact solution to (1.1) at time \(\tilde{t} = \tau_l\) and to emphasize that \(g_{i,j}^0\) is the initial data for (6.2)
or (6.5) at time $\bar{t}_k = \tau_l$ we use the notation $g_{i,j}^0 = g_{i,j}^{0,l}$. Then

$$\text{err}^2(\tau_l) = \left( \frac{\sum_{i,j} (f_e(x_0, v_0, \tau_l) - g_{i,j}^{0,l})^2}{\sum_{i,j} (f_e(x_0, v_0, \tau_l))^2} \right)^{1/2} \left( \frac{c}{(1 - u_{\tau_l}^2)^{3/2}} \Delta u \Delta x \right)^{1/2}$$

$$= \left( \frac{\sum_{i,j} (f_e(x_0, v_0, \tau_l) - g_{i,j}^{0,l})^2}{\sum_{i,j} (f_e(x_0, v_0, \tau_l))^2} \right)^{1/2} \left( \frac{c}{(1 - u_{\tau_l}^2)^{3/2}} \Delta u \Delta x \right)^{1/2}.$$  \hfill (7.2)

The function $f_e(x,v)$ given by (7.1) provides both the initial data for (1.1) for the time dependent computation and also the exact solution, $f_e(x,v,t)$. In (1.1) we let $E(x,t) = E(x) = -c_0(2\pi/L) \sin((2\pi/L)x)$ where $c_0$ is a constant. Then $\phi_0(x)$ in (7.1) is

$$\phi_0(x) = c_0 \left( 1 - \cos \left( \frac{2\pi}{L} x \right) \right)$$  \hfill (7.3)

and $\phi(0) = \phi(L) = 0$. Given the function $\phi_0(x)$ the constant $C$ in (7.1) is computed numerically. To initialize the computation (Section 6.1, part 2(i)) at $\bar{t}_k = 0$, i.e., $l = 0$, $n = 0$, $\tau_l = 0$, $t_0 = 0$, let $g_{i,j}^0 = f_e(x_0, v_0)$, $v_0 = cu_j/\sqrt{1 - u_{\tau}^2}$, $i = 1, \ldots, N_x$, $j = 1, \ldots, N_v$. Then

$$g_{i,j}^{0,0} = g_{i,j}^{0}/\lambda, \quad \lambda = \frac{1}{K} \left( \sum_{i,j} g_{i,j}^{0} \frac{c}{(1 - u_{\tau}^2)^{3/2}} \Delta u \Delta x \right).$$  \hfill (7.4)

with $K$ defined in (7.1). Thus

$$\sum_{i,j} g_{i,j}^{0,0} \frac{c}{(1 - u_{\tau}^2)^{3/2}} \Delta u \Delta x = K.$$  

The initial data are therefore normalized to be consistent with the integral of $f_e(x,v)$ given as

$$\int_{-\infty}^{\infty} f_e(x,v) \, dv \, dx = \int_{0}^{L} \int_{-\infty}^{\infty} f_e(x_0, \sqrt{1 - u_{\tau}^2}) \frac{c}{(1 - u_{\tau}^2)^{3/2}} \, du \, dx_0 = K.$$  

For the exact solution we let

$$f_e(x_0, v_0, \tau_l) = f_e(x_0, v_0) = g_{i,j}^{0,0}$$  \hfill (7.5)

with the grid function $g_{i,j}^{0,0}$ given by (7.4). Thus $f_e(x_0, v_0)$ is obtained by evaluating (7.1) at data points and is then normalized so that the discrete $L_1$ norm has the value $K$.

The numerical method of Section 6 is computed with initial data given by (7.4) and the exact solution given by (7.5). The relative error $\text{err}^2(\tau_l)$ is computed at initialization and regrid times $\tau_l$. If $g_{i,j}^{0,0} = f_e(x_0, v_0)$ at $\tau_l = 0$ then $\text{err}^2(0) = 0$. For the first set of computations we let $\beta = .1$, $q = .002$ in (1.1) and $L = 1$, $K = 3.5$ in (7.1). The parameter, $c$, in (6.1) is $c = .5$. The parameter, $c_0$, in the expression for $\phi_0(x)$, (7.3), is $c_0 = .002$. In the particle computation (Section 6.1, part 2(i)) the approximation of Eq. (2.13) is done by the semi-implicit method (6.2) and by the fully implicit method (6.5). For the present set of parameters the SOR algorithm is used to solve (6.2) and (6.6). A demonstration of the convergence of the numerical method is given in Fig. 1. The graphs of $\text{err}^2$ for the interval $[0,T]$, $T = 10$ are shown for $N_x \times N_v = 50 \times 50$, $\Delta t = .04$, $N_q = 5$; $N_x \times N_v = 70 \times 70$, $\Delta t = .02$, $N_q = 10$; $N_x \times N_v = 100 \times 100$, $\Delta t = .01$, $N_q = 20$; $N_x \times N_v = 140 \times 140$, $\Delta t = .005$, $N_q = 40$. The error $\text{err}^2(\tau_l)$ is plotted at the
regrid times $\tau_l$. The interval of the particle computation is $\tau_{l+1} - \tau_l = \Delta t = N_g \Delta t = .2$ in each case, so the regriding time $\tau_l$ is the same even as the grid parameters $N_x, N_v, \Delta t$ are changed. The solid lines give the graphs for the different grid parameters in which the fully implicit method is used to approximate (2.13), and the broken line graphs show the results using the semi-implicit method to approximate (2.13). It is seen from Fig. 1 that the numerical method of Section 6 is convergent using either the fully implicit or semi-implicit methods for approximating (2.13). Also, as could be expected the computations based on the semi-implicit difference method are slightly less accurate than the computations based on the fully implicit difference method.

Figs. 2 and 3 show a comparison of the grid function $g_{l,j}^{0,l}$ and the exact function $f_e(x_0, cu_j/\sqrt{1 - u_j^2})$ at time $\tau_l = T = 10, l = 50$. Here the computations are based on the semi-implicit differencing with $N_x \times N_v = 100 \times 100, \Delta t = .01, N_g = 20$. In Fig. 2, $x_0$ is fixed and $u_j$ varies on the interval $(-1, 1)$. The solid line is the graph of $f_e(x_0, cu_j/\sqrt{1 - u_j^2})$ and the asterisks give the graph of $g_{l,j}^{0,l}$ with $i = 40, 1 \leq j \leq N_v$. In Fig. 3, $u_j$ is fixed and $x_0$ varies on the interval $(0, 1)$. The graph of $f_e(x_0, cu_j/\sqrt{1 - u_j^2})$ is given by the solid line and the graph of $g_{l,j}^{0,l}$ is given by the dashed line with asterisks with $j = 30, 1 \leq i \leq N_x$. The graphs show that the grid function values $g_{l,j}^{0,l}$ provide a good approximation to the exact function values $f_e(x_0, cu_j/\sqrt{1 - u_j^2})$. The values $g_{l,j}^{0,l}, l = 50$ retain from 3 to 5 significant digits in comparison with the exact values.

The convergence of the numerical procedure of Section 6 is also demonstrated using the Douglas–Rachford method for solving the difference equations (6.2) or (6.5). For these computations some different parameters are used. Let $\beta = .1, q = .1$ in (1.1). The constant $c$ in (6.1) is $c = .2$. The constant $c_0$ in (7.3) is $c_0 = .01$. In (7.1) $L = 1, K = 3.5$ as before. In Fig. 4 the graphs of $err_{l_2}(\tau)$ are shown for $N_x \times N_v = 50 \times 50, \Delta t = .04, N_g = 5; N_x \times N_v = 70 \times 70, \Delta t = .02, N_g = 10; N_x \times N_v = 100 \times 100, \Delta t = .01, N_g = 20; N_x \times N_v = 140 \times 140, \Delta t = .005, N_g = 40$. The solid lines are the graphs for which the fully implicit method (6.5) is used to approximate (2.13), and the broken lines are the graphs for which the semi-implicit method (6.2) is used to approximate (2.13). The convergence of the numerical method is similar to what is seen in Fig. 1.
Figs. 2 and 3 show the comparison of the grid function $g_{i,j}$ and the exact solution $f_e(x_0, cu_j/\sqrt{1 - u_j^2})$ at time $t_T = 10, l = 50$. The computations are based on semi-implicit differencing with $N_x \times N_y = 100 \times 100, \Delta_t = .01, N_x = 20$. In Fig. 5, $x_0$ is fixed and $u_j$ varies with $i = 20, 1 \leq j \leq N_y$. The solid line is the graph of $f_e(x_0, cu_j/\sqrt{1 - u_j^2})$ and
the asterisks the graph of $g_{i,j}^{0,l}$. In Fig. 6, $u_j$ is fixed and $x_0$ varies with $j = 30, 1 \leq i \leq N_x$. The solid line is $f_\varepsilon$, the dashed line with asterisks is $g_{i,j}^{0,l}$. As in the previous example when compared to the exact values the approximate values $g_{i,j}^{0,l}, l = 50$ are accurate to 3 to 5 significant digits.
We would like to correlate the convergence demonstrated numerically with the analytical proofs of convergence given in Sections 4 and 5. The proofs of Sections 4 and 5 are for a simpler model problem and discrete approximation of (1.1). Nonetheless, some relevant comparison can be made with the numerical results. For the partition of phase space as discussed in Section 6.1, part 1 and defined by (3.11) \( \Delta \in L/N_x, \Delta u = 2/(N_t + 1) \). For the examples \( L = 1 \) so for \( N_x, N_t = 50, 70, 100, 140 \) let \( \Delta x_1 = 1/50, \Delta u_1 = 2/100, \Delta x_2 = 1/70, \Delta u_2 = 2/140, \Delta x_3 = 1/100, \Delta u_3 = 2/140, \Delta x_4 = 1/140, \Delta u_4 = 2/140 \).

Then

\[
\Delta x_2 = 5/7 \Delta x_1, \quad \Delta u_2 = 51/70 \Delta u_1, \quad \Delta x_3 = 7/10 \Delta x_2, \quad \Delta u_3 = 71/100 \Delta u_2, \quad \Delta x_4 = 5 \Delta x_3, \quad \Delta u_4 = 101/140 \Delta u_3.
\]

If \( \Delta t_1 = .04, \Delta t_2 = .02, \Delta t_3 = .01, \Delta t_4 = .005 \) then \( \Delta t_2 = .5 \Delta t_1, \Delta t_3 = .5 \Delta t_2, \Delta t_4 = .5 \Delta t_3 \). Let us consider the initial value problem (4.2) and the fully implicit difference approximation (4.3). In this case the coefficients in (4.2), (4.3) are assumed to be known functions, and the discretization is on the whole of phase space. The result of Theorem 4.2 is that the discrete \( L_2 \) error incurred by approximating (4.2) with (4.3) is \( O(\Delta t + (\Delta x)^2 + (\Delta v)^2) \). If we consider for this problem a sequence of discretizations such that

\[
\Delta x_2 = 5/7 \Delta x_1, \quad \Delta v_2 = 51/70 \Delta v_1, \quad \Delta t_2 = .5 \Delta t_1, \\
\Delta x_3 = 7/10 \Delta x_2, \quad \Delta v_3 = 71/100 \Delta v_2, \quad \Delta t_3 = .5 \Delta t_2, \\
\Delta x_4 = 5 \Delta x_3, \quad \Delta v_4 = 101/140 \Delta v_3, \quad \Delta t_4 = .5 \Delta t_3.
\]

Then

\[
\Delta t_{k+1} + (\Delta x_{k+1})^2 + (\Delta v_{k+1})^2 \approx 0.5(\Delta t_k + (\Delta x_k)^2 + (\Delta v_k)^2), \quad k = 1, 2, 3.
\]

Therefore, according to Theorem 4.2 the error of the discrete approximation should reduce by a factor of about \( \mu = .5 \) with each refinement of the phase space grid and the partition of the time interval. However, if the coefficients in the finite difference approximation are not known exactly and need to be approximated numerically then we follow the result of Theorem 5.1. Also, in Theorem 5.1 the discretization does not cover all of space but is carried out on a finite domain. The result of Theorem 5.1 indicates that the reduction in the error with a refinement of the grid may be less than what is predicted by Theorem 4.2. According to Theorem 5.1 for a fixed small parameter, \( \varepsilon_1 \), then there is an
$R_0 = R_0(\epsilon_1)$ which is sufficiently large so that the quantity $R(g(\cdot, t_n))$ defined by (5.35) is such that $\|R(g(\cdot, t_n))\| < \epsilon_1$ for $0 \leq t_n \leq T$. Then there is a constant $C(R_0(\epsilon_1), T)$ such that the discrete $L_2$ error in approximating (2.7) by (5.22) is given by (5.38). It is convenient to put this estimate into the form

$$\|\varepsilon^0\| \leq C(R_0(\epsilon), T) ((\Delta x)^2 + (\Delta v)^2 + \Delta t) + C(T) \epsilon_1$$

with the assumption that $C(R_0(\epsilon), T) \geq C(T)$. We let $C(T) \epsilon_1 = \epsilon$ and $\Delta = (\Delta x)^2 + (\Delta v)^2 + \Delta t$ and write

$$\|\varepsilon^0\| \leq C(R_0(\epsilon), T) \Delta + \epsilon = CA + \epsilon.$$  \hspace{1cm} (7.6)

With this estimate for the error a refinement of the grid as given above does not result in a reduction of the error by factor of $\mu \approx .5$ but by some factor $\mu > .5$. Let $A_1 = (\Delta x_1)^2 + (\Delta v_1)^2 + \Delta t_1$ and $A_2 = (\Delta x_2)^2 + (\Delta v_2)^2 + \Delta t_2$ and assume $A_2 = .5A_1$ then

$$\frac{C \mu A_2 + \epsilon}{C \mu A_1 + \epsilon} = \frac{\frac{1}{2} C A_1 + \epsilon}{C A_1 + \epsilon} = \mu$$ \hspace{1cm} (7.7)

and $\frac{1}{2} < \mu < 1$. The parameter, $\epsilon$, is a measure of the error incurred by replacing the infinite domain by a finite domain for the discrete approximation. The parameter, $R_0$, is a measure of the size of the finite domain. The smaller $\epsilon$ is relative to $A_1$, the closer $\mu$ is to $.5$. If $\epsilon$ is fixed and $A_1$ decreases then $\mu$ increases.

We look for some correspondence between the theoretical result of Theorem 5.1 and the computational results of Section 7.1. The convergence result of Fig. 1 is considered. Here $\beta = .1$, $q = .002$, $c_0 = .002$, and the SOR method is used in the finite difference approximation of (2.13). For the case where the fully implicit method is used for approximating (2.13) Table 2 gives the values $\text{errl}_2(\tau_i) = \text{errl}_2(n)$ at $\tau_i = 10$ as the mesh parameters $\Delta x$, $\Delta u$, $\Delta t$ are refined. The index $n$ is a reference number for the refinement. It is seen that $\text{errl}_2$ decreases as expected as the mesh is refined but the ratio $\text{errl}_2(n)/\text{errl}_2(n-1)$ increases. This can correspond to the case where $\epsilon$ in the error estimate (7.6) is a significantly large quantity in relation to $A$. To make $\epsilon$ less significant in the estimate (7.6) one can widen the grid for the discrete approximation. That is the parameter $\epsilon_1$ and also $\epsilon = C(T) \epsilon_1$ is reduced and $R_0(\epsilon_1)$ is increased, which can also increase the constant $C(R_0(\epsilon_1))$. The ratio $\mu$ given by (7.7) should then be closer to $.5$. There is not an exact parallel between the partition of phase space for Theorem 5.1 and the numerical method of Section 6. For Theorem 5.1 there is a uniform cut-off parameter independent of $\Delta x$, $\Delta v$ given by $R_0$ which defines the domain of the discrete problem. For the periodic problem being solved by the numerical method of Section 6 the domain is infinite in velocity space, and there is no uniform cut-off parameter for the partition of velocity space given by (6.1). In (6.1) the parameter $c$ adjusts the width of the domain of the discrete problem in velocity space. Increasing $c$ widens the grid in velocity space and may have a similar result as reducing $\epsilon_1$ and increasing $R_0(\epsilon_1)$ in the context of the discretization of Theorem 5.1. We, therefore, see what the effect is of making $c$ larger. For the computations of Table 2 $c = .5$ in (6.1). This constraint is now set to $c = 2$, and the computations of Table 2 are repeated with the larger value of $c$. The result is given in Table 3. First what is noted is that the discrete $L_2$ error at $T = 10$ given by $\text{errl}_2(n)$ is significantly greater than in Table 2. What is also apparent is that the ratios $\text{errl}_2(n)/\text{errl}_2(n-1)$ are much closer to $.5$. Thus, we can conjecture that the error estimate for approximating the periodic problem has a form in terms of $\Delta x$, $\Delta u$, $\Delta t$ analogous to (7.6) and that widening the grid in velocity space has an effect similar to increasing $R_0$ and decreasing $\epsilon$ in the error estimate (7.6). That is the contribution to the error from truncating the domain is made small compared to the contribution to the error from discretizing the domain. A similar result is obtained for computations based on the Douglas–Rachford method as given in Fig. 4. For the computations in Fig. 4, $c = 2$ in (6.1), and the ratios of $\text{errl}_2(n)$ at $T = 10$ increase as discretization parameters.
7.2. Time dependent approach to steady state

For initial data which is not a steady state solution to (1.1) the numerical method of Section 6 is applied to demonstrate the convergence to the steady state as time, \( t \), increases. The computations verify the result of [3, Theorem A] in the context of the present 1-D periodic problem.

In computing the approach to steady state we consider the graphs of kinetic energy and free energy. The steady state value of these quantities can be derived from the function (7.1). To derive the steady state value of kinetic energy the function \( f(x,v,t) \) in the expression for kinetic energy, [19, Section 2.4], is replaced with (7.1). Thus

\[
\frac{1}{2} \int_0^L \int_{-\infty}^\infty v^2 f_s(x,v) \, dv \, dx = \frac{1}{2} K \left( \int_{-\infty}^{\infty} \frac{v^2}{\sqrt{2\pi(q/\beta)}} \exp \left( -\frac{v^2}{2q/\beta} \right) \, dv \right) \left( \frac{1}{C} \int_0^L \exp \left( -\frac{\phi_0(x)}{q/\beta} \right) \, dx \right)
\]

\[
= \frac{K(q/\beta)}{2}.
\]

Therefore, as \( t \to \infty \) then

\[
\text{ke}(t) \to \frac{K(q/\beta)}{2}.
\]  

(7.8)

The free energy, \( \text{FE} \), is given by \( \text{FE}(t) = \text{ke}(t) + \text{pe}(t) - q/\beta \text{ent}(t) \) where the potential energy, \( \text{pe}(t) \), is given by (6.3), and the entropy, \( \text{ent}(t) \), is defined in [19, Section 2.4]. Replacing \( f(x,v,T) \) with (7.1) in the expression for entropy in [19, Section 2.4] one obtains

\[
- \int_0^L \int_{-\infty}^\infty f_s(x,v) \ln(f_s(x,v)) \, dv \, dx
\]

\[
= - \int_0^L \int_{-\infty}^\infty \frac{K}{C\sqrt{2\pi(q/\beta)}} \exp \left( -\frac{v^2}{2q/\beta} \right) \exp \left( -\frac{\phi_0(x)}{q/\beta} \right) \left( \ln \left( \frac{K}{C\sqrt{2\pi(q/\beta)}} \right) - \frac{v^2}{2q/\beta} - \frac{\phi_0(x)}{q/\beta} \right) \, dv \, dx
\]

\[
= -K \ln \left( \frac{K}{C\sqrt{2\pi(q/\beta)}} \right) + K/2 + KD,
\]

where

\[
D = \frac{1}{C} \int_0^L \frac{\phi_0(x)}{q/\beta} \exp \left( -\frac{\phi_0(x)}{q/\beta} \right) \, dx.
\]
Thus, as \( t \to \infty \), \( \Delta t \to 0 \), we find that for larger \( q \) values the more \( q/\beta K D \) converges. For \( \beta > 0 \) fixed then as \( q \) increases the rates of convergence of the iterative methods for solving (6.2) decrease. This is seen in the proof of convergence of the Jacobi method. The Jacobi method for the field free case is stated as (3.17). For nonzero electric field this iterative procedure is stated as [19, (2.5)]. The method is shown to converge because \( \Theta(t_n) \) given for the field free case following (3.17), is such that \( 0 < \Theta(t_n) < 1 \). With nonzero electric field this quantity is given in [19] as

\[
\Theta(t_n) = \max_{i,j} \left( \frac{2qr_1a_{i,j}^2(t_n) + qr_2b_{i,j}^2(t_n)s_j(s_j^1 + s_j^0)}{D_{i,j}} \right)
\]

with \( D_{i,j} = 1 + 2qr_1a_{i,j}^2(t_n) + qr_2b_{i,j}^2(t_n)s_j(s_j^1 + s_j^0) \). The quantities \( s_j, s_j^1, s_j^0 \) are defined by (3.12). For fixed parameters \( \Delta x, \Delta u, \Delta t \) and given coefficients \( a_{i,j}(t_n), b_{i,j}(t_n) \) then as \( q \) increases \( \Theta(t_n) \to 1 \). The closer \( \Theta(t_n) \) gets to one the slower the convergence of the Jacobi method, and similarly the more iterations required for convergence of the SOR method. With the slower convergence of the SOR method for increasing \( q \) we find that for larger \( q \) values the more efficient method for solving (6.2) is the direct Douglas–Rachford method. The Douglas–Rachford method for nonzero electric field is stated as [19, (2.11), (2.12)]. In this method first \( N_\ell \) linear equations in \( N_\ell \) unknowns must be solved \( N_\ell \) times followed by \( N_\ell \) linear equations in \( N_\ell \) unknowns to be solved \( N_\ell \) times. It is to be noted that the \( N_\ell \) equations in \( N_\ell \) unknowns has a coefficient matrix that is tridiagonal, and the speed of computation of the Douglas–Rachford method is significantly increased by using a system solver that takes account of this structure.

The constant \( c_0 = 0.002 \). The parameter \( \beta \) in (1.1) also remains fixed with \( \beta = .1 \). The computations are then carried out on a time interval \([0, T]\) for values \( q \) increasing from 0.0001 to 100. For \( q = 0.0001 \) then \( T = 100 \). For other \( q \) values \( T = 50 \). With \( \beta \) and \( c_0 \) fixed then as \( q \) increases the steady state value of \( ke \) increases. As a function of \( q \) the steady state \( FE \) increases for small \( q \), attains a maximum value around \( q = 0.07 \), then decreases with \( FE = 0 \) around \( q = 0.2 \). Further increasing \( q \) then \( FE \) becomes negative and continues to decrease as \( q \) increases.
Table 4 shows the values of free energy as a function of $q$. The FE values computed at times $t = 0$, FE$_0$ and $t = T$, FE$_T$ are compared to the steady state value of FE computed from (7.9), given by FE$_S$.

A characteristic of the computations of Table 4 is that with increasing $q$ the diffusion in velocity space becomes a more pronounced effect. As a result it becomes necessary to increase the number of discrete velocities in the initial particle distribution, particularly the number of higher velocity particles, in order to obtain a sufficiently accurate solution. A way of doing this without increasing the total number, $N$, of data points is to let $N_v > N_x$ with $N_x N_v = N$. It is found that good accuracy can be attained this way using a relatively coarse grid in the $x$-variable. In addition, with increasing $N_v$ the constant $c$ in (6.1) can be increased which widens the domain in velocity space. If additional accuracy is still required the total number of particles, $N$, is increased. With increasing $q$ and increasing number of data points in the computation and with $N_v > N_x$ the computing time for Douglas–Rachford becomes significantly less than for SOR. Thus, in Table 4 the SOR method for solving (6.2) is used for $q = .0001, .001$, and the Douglas–Rachford method is

<table>
<thead>
<tr>
<th>$q$</th>
<th>$N_x \times N_v$</th>
<th>$N_y$</th>
<th>$c$</th>
<th>FE$_0$</th>
<th>FE$_T$</th>
<th>FE$_S$</th>
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<tr>
<td>0.0001</td>
<td>100 $\times$ 100</td>
<td>400</td>
<td>.5</td>
<td>0.030527</td>
<td>0.017377</td>
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<td>100</td>
<td>.5</td>
<td>.099280</td>
<td>0.098927</td>
<td>0.098925</td>
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<td>50 $\times$ 200</td>
<td>100</td>
<td>.5</td>
<td>.786808</td>
<td>0.526759</td>
<td>0.526756</td>
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<tr>
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<td>25 $\times$ 400</td>
<td>100</td>
<td>1</td>
<td>5.37032</td>
<td>1.261799</td>
<td>1.261792</td>
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<td>1</td>
<td>7.66208</td>
<td>1.175408</td>
<td>1.175382</td>
</tr>
<tr>
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<td>100</td>
<td>1</td>
<td>15.3013</td>
<td>–0.081793</td>
<td>–0.082246</td>
</tr>
<tr>
<td>0.4</td>
<td>25 $\times$ 800</td>
<td>100</td>
<td>2</td>
<td>30.5797</td>
<td>–5.023503</td>
<td>–5.023519</td>
</tr>
<tr>
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<td>2</td>
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<td>8</td>
<td>7639.22</td>
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<td>–10920.18</td>
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</table>

$^a$For $q = .0001$, $T = 100$, for $q \geq .001$, $T = 50$, $\Delta t = .01$.  

Fig. 7. beta = 0.1, $c_0 = 0.002$, dt = 0.01.
used for $q \geq 0.1$. For all computations $\Delta t = 0.01$. It can be noted that for large $q$ values the change in FE from $t = 0$ to the steady state is very large. Table 4 shows that a good accuracy is attained for the approach to the steady state value of FE for a wide range of the diffusion parameter $q$.

Graphs of $k_e$ and FE are shown in Figs. 7–9. The steady state value of $k_e$ is given by (7.8). With $K = 3.5$, $\beta = 0.1$ then for $q = 0.1, 0.2, 0.4$ the graphs of $2k_e$ approach steady state values of 3.5, 7, 14, respectively. These graphs are
shown in Fig. 7. The corresponding FE graphs are contained in Fig. 8 for the time interval $[0, 15]$. The free energy is a monotonically decreasing function of time as is proved in [3]. The steady state value of FE is given by (7.9). The FE graph for $q = .4$ is shown on a fine scale in Fig. 9. The jumps in this graph are discontinuities resulting from the regridding. The regridding process discussed in Section 6.1, part 3 preserves the continuity of the kinetic energy but not that of potential energy or entropy. Hence, on the fine scale the free energy shows the discontinuities at points of regridding.

8. Summary and conclusion

In this paper we have applied the numerical method described in [19] to the linear Vlasov–Fokker–Planck equation in one dimension. Here the electric field is a known external force and is not computed to be internally consistent with the phase space distribution function. For this linear equation some of the problems of stability and convergence of the numerical method of [19] are addressed. More specifically a main aspect of the numerical method of [19] is to transform Eq. (1.1) based on integrals of the characteristic. The transformed equation is then approximated by a finite difference method. The analysis in the present paper studies the stability and accuracy of this finite difference approximation. First, Eq. (1.1) is considered for which $E(x, t) = 0$. For the analysis of stability and convergence the initial value problem in all space is studied. The transformation based on integrals of the characteristic equations puts Eq. (2.19) into the form (2.25) in which the coefficients are known functions of $t$. A semi-implicit difference method is applied to approximate the solution to (2.25). It is proved based on Fourier transform methods that this semi-implicit method is unconditionally stable and convergent. For the purpose of computation Eq. (2.25) is further transformed to the form (2.26), and periodic boundary conditions are introduced. The semi-implicit difference method is then adapted to this periodic, boundary value problem as (3.15). Two methods for solving (3.15) are introduced, the iterative SOR algorithm and the direct Douglas–Rachford method. Some problems regarding the convergence and implementation of the SOR algorithm are addressed through a computation of the eigenvalues of the transformation associated with the iterative procedure. The unconditional stability of the Douglas–Rachford procedure is proved in the context of the initial value problem.

When the external field, $E(x, t)$, in (1.1) is not zero the transformed equation for the initial value problem, which is given by (2.7), has coefficients which depend on the spatial and velocity variables as well as $t$. For the analysis of stability and convergence of the finite difference approximation to (2.7) we cannot depend on the Fourier transform techniques. Nevertheless, in Section 4 it is proved that a fully implicit finite difference approximation to (2.7) is unconditionally stable and convergent. It is assumed in the proof of Section 4 that the coefficients in the fully implicit difference equation (4.3) are known functions. However, in practice these functions are not known exactly and must be obtained by numerically approximating the solutions to the trajectory equations along with approximations of the first and second partial derivatives of these trajectories. The inclusion of the computation of the trajectories gives a numerical method which can be viewed as a type of deterministic particle method. In Section 5 a theorem is proved which guarantees the convergence of the fully implicit difference method with approximate coefficients to the solution of the initial value problem (2.7). This constitutes proving the convergence of the deterministic particle method to the solution of the initial value problem (2.1). The fully implicit difference method with approximate coefficients is adapted to solve the periodic, boundary value problem (2.13). This then is the main part of the deterministic particle method described in Section 6 for approximating the solution to the periodic, boundary value problem (1.1). A numerical verification of convergence of the deterministic particle method and a comparison of the semi-implicit and fully implicit methods for approximating (2.13) is carried out in Section 7.1. It is determined computationally that both the fully implicit and semi-implicit methods for approximating (2.13) give a convergent numerical method, and there is not a significant difference between solutions computed with the fully implicit method and those computed with the semi-implicit method. The theoretical results of Sections 4 and 5 provide proofs of convergence that apply to a fully implicit difference method; however, as the computational work shows the numerical method based on semi-implicit differencing converges to the same solution as with fully implicit differencing. This comparison along with the results of Sections 4 and 5 provides some theoretical verification of the semi-implicit method which is the preferred method for approximating (2.13).

From the numerical work of Section 7.2 we demonstrate that with the deterministic particle method we can compute an accurate solution to (1.1) for a wide range of the parameter determining the Fokker–Planck diffusion. The computed solution converges to a steady state which is consistent with the time asymptotic solution proved analytically in [3, Theorem A].
Acknowledgments

We would like to thank the referees for comments and suggestions that have contributed to this paper.

References


Further reading