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Hamilton's Principle and Numerical
Solution of the Vlasov Equations

UNITED STATES
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Printed in the United States of America. Available from
Clearinghouse for Federal Scientific and Technical Information
National Bureau of Standards, U. S. Department of Commerce
Springfield, Virginia 22151

Price: Printed Copy \$3.00; Microfiche \$0.65

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of the
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Report written: October 1967

Report distributed: September 13, 1968

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H. Ralph Lewis

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HAMILTON'S PRINCIPLE AND NUMERICAL SOLUTION OF THE VLASOV EQUATIONS

by

H. Ralph Lewis

ABSTRACT

It is demonstrated how Hamilton's principle can be used to derive equations that approximate the Vlasov integro-partial differential equations. The Lagrangian that is used is sufficiently general to describe physical systems in which there are present any of a large class of material media that exhibit nonlinear polarizability and magnetizability. The aim is to obtain useful approximate equations that are more convenient for numerical solution than the exact integro-partial differential equations. The approximate equations that are emphasized are a system of ordinary differential equations in time, although the basic method can be used to derive other approximate equations, such as a system of difference equations. The basic method can be applied to any Lagrangian system. The equations for a simple, one-dimensional example are displayed explicitly.

I. INTRODUCTION

The Vlasov system of integro-partial differential equations, expressed in terms of Lagrangian variables for the particles and Eulerian variables for the electromagnetic field, can be derived from Hamilton's principle by using the Lagrangian given by Low¹ and Sturrock.² That Lagrangian can be generalized to include systems in which there are present any of a large class of material media that exhibit nonlinear polarizability and magnetizability, and also to include nonelectromagnetic forces. These possibilities allow convenient imposition of certain kinds of particle and field boundary conditions for finite systems. In this report we demonstrate how Hamilton's principle can also be used to derive equations for these systems that approx-

imate the exact equations of motion. The aim is to obtain useful approximate equations that are more convenient for numerical solution than the exact integro-partial differential equations. The approximate equations that we shall emphasize are a system of ordinary differential equations in time, although the basic method can be used to derive other approximate equations, such as a system of difference equations. The basic method can be applied to any Lagrangian system.

The first step in solving equations approximately by any method is to choose the form in which the desired functions are to be represented. A common way of representing a function of continuous variables approximately is to specify the function

on a mesh; that is, to specify the function at each of a set of discrete values of the arguments. Another method of representation that is frequently used is to approximate the function by a linear combination of a finite number of linearly independent basis functions. The representation that we choose is a combination of these two, because we shall derive differential equations in time that must generally be solved numerically, whereas the dependences of the unknown functions on other variables will be represented by linear combinations of linearly independent basis functions. Let $g(x,t)$ be one of the functions to be represented, where t denotes time and x denotes the remaining arguments of g . For each particular value of t , we approximate $g(x,t)$ by a linear combination of a finite number of linearly independent basis functions which we may call $\psi_i(x)$. The coefficients in the expansion are functions of t only, so that the representation of $g(x,t)$ is

$$g(x,t) = \sum_{i=1}^N a_i(t) \psi_i(x). \quad (1)$$

If we choose to approximate all of the unknown functions in this fashion, the problem then is to derive equations that determine the time evolution of the time-dependent coefficients and to solve those equations. The differential equations that are chosen to determine the time evolution of the coefficients will be ordinary differential equations, and, from the standpoint of numerical analysis, that in itself may provide a distinct advantage over working with a system of integro-partial differential equations. By choosing the basis functions appropriately, we can bring the system of ordinary differential equations into a form for which there are standard finite-difference methods whose properties are relatively well understood. At least one such method is formulated in a way that guarantees numerical stability.^{3,4}

Requiring that the unknown functions be approximated as illustrated by Eq. (1) does not specify the differential equations that determine the time evolution of the coefficients. In fact, there are infinitely many systems of equations for the coefficients that can be derived from the exact integro-differential equations. The solutions of these dif-

ferent systems will differ in the fidelity with which they represent the time evolution of the unknown functions, and it is desirable to have a criterion for choosing one of the infinitude of systems. The method that we propose for choosing a system is to substitute the approximate representations of the unknown functions into the Lagrangian density and then determine the system of differential equations for the time-dependent coefficients by applying Hamilton's principle. The only difference between this procedure and using Hamilton's principle to derive the exact equations is that the functional variations are restricted to be within the class of functions that we have chosen for approximating the unknown functions; the variation of the integral of the Lagrangian is made to vanish exactly. In some useful sense the system of equations so derived should approximate the exact equations as well as is possible, given the particular scheme that was chosen for approximating the functions.

It is hoped that this procedure based on Hamilton's principle will prove advantageous for nonlinear systems, such as the Vlasov equations, and that some useful properties of the approximate system of equations can be derived.

In Section II we begin the exposition by defining the physical system and deriving the exact equations of motion from Hamilton's principle. The derivation of the exact equations, although standard for the most part, is carried out in detail so as to provide a firm basis for the derivation of approximate equations. Particular attention is given to the boundary conditions that must be imposed on the functions and their variations. The derivation of approximate equations is described in Section III for orthogonal coordinate systems, and details are given for cartesian, cylindrical, and toroidal coordinates. The equations are displayed explicitly for a simple, one-dimensional example in Section IV. Work is underway to solve the approximate equations for this example numerically.

II. THE PHYSICAL SYSTEM, THE LAGRANGIAN, AND HAMILTON'S PRINCIPLE

A. The Physical System

We consider a collection of charged particles consisting of N distinct species. The masses and

charges of the individual particles are, respectively, m_i and q_i ($i = 1, \dots, N$). These particles interact with one another through the electromagnetic field, and they may also be acted on by nonelectromagnetic forces. The behavior of the particles of each species is described by a distribution function for that species. For species i the distribution function is written as $f_i(\underline{r}, \underline{v}, t)$, where $\underline{r}$ is the position vector, $\underline{v}$ is velocity, and t is time. The sources of the electromagnetic field consist of external (prescribed) sources plus sources determined by average behavior of the charged particles. The charge and current densities, $\rho(\underline{r}, t)$ and $\underline{j}(\underline{r}, t)$, are

$$\left. \begin{aligned} \rho(\underline{r}, t) &= \rho_0(\underline{r}, t) + \sum_{i=1}^N q_i \int f_i(\underline{r}, \underline{v}, t) d^3 \underline{v} \\ \underline{j}(\underline{r}, t) &= \underline{j}_0(\underline{r}, t) + \sum_{i=1}^N q_i \int \underline{v} f_i(\underline{r}, \underline{v}, t) d^3 \underline{v} \end{aligned} \right\} \quad (2)$$

where $\rho_0(\underline{r}, t)$ and $\underline{j}_0(\underline{r}, t)$ are the external sources.

In addition to describing the particles by distribution functions, we also follow the individual particles as they move according to Newton's law as a result of being acted on by the averaged electromagnetic field whose sources are given by Eqs. (2), and by the nonelectromagnetic force field, if any. Explicit use of the individual particle description is made in the Lagrangian formulation of Low¹ and Sturrock.² We denote the position vector of a particle of species i , whose initial position vector and velocity are $\underline{r}'$ and $\underline{v}'$, by $\underline{R}_i(\underline{r}', \underline{v}', t)$. The equations satisfied by these functions are

$$\begin{aligned} m_i \frac{\partial^2 \underline{R}_i}{\partial t^2} &= q_i \left[\underline{E}(\underline{R}_i, t) + \frac{1}{c} \frac{\partial \underline{R}_i}{\partial t} \times \underline{B}(\underline{R}_i, t) \right] \\ &+ \underline{F}_i(\underline{R}_i, \dot{\underline{R}}_i, t), \quad i = 1, \dots, N, \end{aligned} \quad (3)$$

where c is the speed of light, $\underline{E}$ is the electric field, $\underline{B}$ is the magnetic field, $\dot{\underline{R}}_i$ is $\partial \underline{R}_i / \partial t$, and $\underline{F}_i$ is a nonelectromagnetic force. The nonelectromagnetic force may be velocity dependent, but we assume that it can be derived from a generalized potential, $U_i(\underline{R}_i, \dot{\underline{R}}_i, t)$, according to the relation

$$\underline{F}_i(\underline{R}_i, \dot{\underline{R}}_i, t) = - \nabla_{\underline{R}_i} U_i(\underline{R}_i, \dot{\underline{R}}_i, t) + \frac{d}{dt} \left[\nabla_{\dot{\underline{R}}_i} U_i(\underline{R}_i, \dot{\underline{R}}_i, t) \right]. \quad (4)$$

The initial conditions on $\underline{R}_i(\underline{r}', \underline{v}', t)$ are

$$\left. \begin{aligned} \underline{R}_i(\underline{r}', \underline{v}', 0) &= \underline{r}' \\ \dot{\underline{R}}_i(\underline{r}', \underline{v}', 0) &= \underline{v}' \end{aligned} \right\} \quad (5)$$

We describe the electromagnetic field for the case in which polarizable and magnetizable material media may be present; that is, we write Maxwell's equations as

$$\left. \begin{aligned} \nabla \cdot \underline{B} &= 0 \\ \nabla \times \underline{E} &= - \frac{1}{c} \frac{\partial \underline{B}}{\partial t} \\ \nabla \cdot \underline{D} &= 4\pi \rho \\ \nabla \times \underline{H} &= \frac{4\pi}{c} \underline{j} + \frac{1}{c} \frac{\partial \underline{D}}{\partial t} \end{aligned} \right\} \quad (6)$$

The vectors $\underline{D}$ and $\underline{H}$ are to be derivable from two scalar functions, $\psi(\underline{E}, \underline{r}, t)$ and $\chi(\underline{B}, \underline{r}, t)$, by means of the formulas

$$\left. \begin{aligned} \underline{D}(\underline{r}, t) &= 4\pi \nabla_{\underline{E}} \psi(\underline{E}, \underline{r}, t) \\ \underline{H}(\underline{r}, t) &= 4\pi \nabla_{\underline{B}} \chi(\underline{B}, \underline{r}, t) \end{aligned} \right\} \quad (7)$$

These formulas admit a large class of nonlinear relations between the vectors $\underline{D}$ and $\underline{H}$ and the vectors $\underline{E}$ and $\underline{B}$. The functions ψ and χ depend on $\underline{r}$ and t implicitly through the dependence on $\underline{E}$ and $\underline{B}$. In addition to this implicit dependence, explicit dependence on $\underline{r}$ and t is also allowed. As a result, ψ and χ can be used to describe situations in which the nature and distribution of polarizable and magnetizable material media change spatially and temporally. It may be feasible to use this feature in plasma problems for locating material boundaries for the electromagnetic field. However, in regions where particles are allowed, we would normally take $\psi = E^2/8\pi$ and $\chi = B^2/8\pi$, so that $\underline{D}$ and $\underline{H}$ are given by $\underline{D} = \underline{E}$ and $\underline{H} = \underline{B}$. A possible exception to this would arise if the plasma were described by a dielectric coefficient. The generality of the functions ψ and χ is probably most useful in problems of nonlinear optics.

We introduce scalar and vector potentials, $\phi(\underline{r}, t)$ and $\underline{A}(\underline{r}, t)$, in the standard way by the relations

$$\left. \begin{aligned} \underline{\underline{B}} &= \nabla \times \underline{\underline{A}} \\ \underline{\underline{E}} &= -\nabla\varphi - \frac{1}{c} \frac{\partial \underline{\underline{A}}}{\partial t} \end{aligned} \right\} \quad (8)$$

When the scalar and vector potentials are used, the first two of Eqs. (6) are satisfied automatically.

B. Derivation of the Exact Equations of Motion from Hamilton's Principle

The Lagrangian for the physical system defined by Eqs. (2)-(8) is

$$\begin{aligned} L = & \sum_{i=1}^N \int d^3 \underline{\underline{r}}' d^3 \underline{\underline{v}}' f_i(\underline{\underline{r}}', \underline{\underline{v}}', 0) \left\{ \frac{1}{2} m_i \left(\frac{\partial \underline{\underline{R}}_i}{\partial t} \right)^2 - U_i(\underline{\underline{R}}_i, \underline{\underline{R}}_i, t) \right. \\ & \left. - q_i \varphi(\underline{\underline{R}}_i, t) + \frac{1}{c} q_i \frac{\partial \underline{\underline{R}}_i}{\partial t} \cdot \underline{\underline{A}}(\underline{\underline{R}}_i, t) \right\} \\ & + \int_V d^3 \underline{\underline{r}} \left\{ \psi(\underline{\underline{E}}, \underline{\underline{r}}, t) - \chi(\underline{\underline{B}}, \underline{\underline{r}}, t) - \rho_o(\underline{\underline{r}}, t) \varphi(\underline{\underline{r}}, t) \right. \\ & \left. + \frac{1}{c} \underline{\underline{j}}_o(\underline{\underline{r}}, t) \cdot \underline{\underline{A}}(\underline{\underline{r}}, t) \right\}. \quad (9) \end{aligned}$$

The integration over $\underline{\underline{r}}'$ and $\underline{\underline{v}}'$ extends over the full range of these variables. The integration over $\underline{\underline{r}}$ extends over a volume, V , on whose boundaries appropriate boundary conditions on the electromagnetic field have been prescribed. The vectors $\underline{\underline{E}}$ and $\underline{\underline{B}}$ are to be expressed in terms of φ and $\underline{\underline{A}}$ by Eqs. (8). The exact equations of motion for the system can be derived from Hamilton's principle,

$$\delta \int_{t_1}^{t_2} L dt = 0, \quad (10)$$

where the functions to be varied independently are φ , $\underline{\underline{A}}$, and the $\underline{\underline{R}}_i$. During the course of our derivation of the equations of motion it will become clear what restrictions must be placed on the class of functions in which φ , $\underline{\underline{A}}$, and the $\underline{\underline{R}}_i$ are to be varied. Certain boundary conditions must be prescribed, and it must be assumed that the $\underline{\underline{R}}_i$ and the component of $\underline{\underline{A}}$ along $\underline{\underline{D}}$ assume prescribed values at times t_1 and t_2 . Requiring the $\underline{\underline{R}}_i$ and the component of $\underline{\underline{A}}$ along $\underline{\underline{D}}$ to assume prescribed values at times t_1 and t_2 is equivalent to prescribing the $\underline{\underline{R}}_i$ and $\underline{\underline{R}}_i$ and the components of $\underline{\underline{A}}$ and $\dot{\underline{\underline{A}}}$ along $\underline{\underline{D}}$ at time t_1 . The reason is that specification of these quantities at a single time determines a unique solution.

The variation of the integral of the Lagrangian with respect to $\underline{\underline{R}}_k$ is

$$\begin{aligned} \delta_{\underline{\underline{R}}_k} \int_{t_1}^{t_2} L dt = & \int_{t_1}^{t_2} dt \int d^3 \underline{\underline{r}}' d^3 \underline{\underline{v}}' f_k(\underline{\underline{r}}', \underline{\underline{v}}', 0) \left\{ \left[-\nabla_{\underline{\underline{R}}_k} U_k(\underline{\underline{R}}_k, \underline{\underline{R}}_k, t) \right. \right. \\ & \left. - q_k \nabla_{\underline{\underline{R}}_k} \varphi(\underline{\underline{R}}_k, t) + \frac{1}{c} q_k \left(\nabla_{\underline{\underline{R}}_k} \underline{\underline{A}}(\underline{\underline{R}}_k, t) \right) \cdot \underline{\underline{R}}_k \right] \cdot \delta \underline{\underline{R}}_k \\ & \left. + \left[m_k \underline{\underline{R}}_k - \nabla_{\underline{\underline{R}}_k} U_k(\underline{\underline{R}}_k, \underline{\underline{R}}_k, t) + \frac{1}{c} q_k \underline{\underline{A}}(\underline{\underline{R}}_k, t) \right] \cdot \delta \underline{\underline{R}}_k \right\} \\ = & \int_{t_1}^{t_2} dt \int d^3 \underline{\underline{r}}' d^3 \underline{\underline{v}}' f_k(\underline{\underline{r}}', \underline{\underline{v}}', 0) \left\{ m_k \underline{\underline{R}}_k - \nabla_{\underline{\underline{R}}_k} U_k(\underline{\underline{R}}_k, \underline{\underline{R}}_k, t) \right. \\ & \left. + \frac{d}{dt} \nabla_{\underline{\underline{R}}_k} U_k(\underline{\underline{R}}_k, \underline{\underline{R}}_k, t) - q_k \nabla_{\underline{\underline{R}}_k} \varphi(\underline{\underline{R}}_k, t) - \frac{1}{c} q_k \underline{\underline{A}}(\underline{\underline{R}}_k, t) \right. \\ & \left. + \frac{1}{c} q_k \left[\nabla_{\underline{\underline{R}}_k} \underline{\underline{A}}(\underline{\underline{R}}_k, t) \cdot \underline{\underline{R}}_k - \underline{\underline{R}}_k \cdot \nabla_{\underline{\underline{R}}_k} \underline{\underline{A}}(\underline{\underline{R}}_k, t) \right] \right\} \cdot \delta \underline{\underline{R}}_k, \quad (11) \end{aligned}$$

where, as before, the dot denotes partial differentiation with respect to time. Here we have required

$$\left[m_k \underline{\underline{R}}_k - \nabla_{\underline{\underline{R}}_k} U_k(\underline{\underline{R}}_k, \underline{\underline{R}}_k, t) + \frac{1}{c} q_k \underline{\underline{A}}(\underline{\underline{R}}_k, t) \right] \cdot \delta \underline{\underline{R}}_k \Big|_{t_1}^{t_2} = 0, \quad (11a)$$

and, in order to satisfy this condition generally, we require

$$\delta \underline{\underline{R}}_k = 0 \quad \text{for } t = t_1 \text{ and } t_2.$$

This is the same as giving $\underline{\underline{R}}_k$ prescribed values at times t_1 and t_2 . Since the right-hand side of Eq. (11) must vanish for arbitrary $\delta \underline{\underline{R}}_k$ that vanish at times t_1 and t_2 , the part of the integrand within the curly brackets in Eq. (11) must itself vanish. By using the relation

$$(\nabla_{\underline{\underline{R}}_k} \underline{\underline{A}}) \cdot \underline{\underline{R}}_k - \underline{\underline{R}}_k \cdot (\nabla_{\underline{\underline{R}}_k} \underline{\underline{A}}) = \underline{\underline{R}}_k \times (\nabla_{\underline{\underline{R}}_k} \times \underline{\underline{A}}), \quad (11b)$$

along with Eqs. (4) and (8), we obtain Eq. (3).

Varying the integral of the Lagrangian with respect to φ , we obtain

$$\begin{aligned} \delta_{\varphi} \int_{t_1}^{t_2} L dt = & - \sum_{i=1}^N \int_{t_1}^{t_2} dt \int d^3 \underline{\underline{r}}' d^3 \underline{\underline{v}}' f_i(\underline{\underline{r}}', \underline{\underline{v}}', 0) q_i \delta \varphi(\underline{\underline{R}}_i, t) \\ & + \int_{t_1}^{t_2} dt \int_V d^3 \underline{\underline{r}} \left\{ -[\nabla_{\underline{\underline{E}}} \psi(\underline{\underline{E}}, \underline{\underline{r}}, t)] \cdot \delta [\nabla_{\underline{\underline{E}}} \varphi(\underline{\underline{r}}, t)] - \rho_o(\underline{\underline{r}}, t) \delta \varphi(\underline{\underline{r}}, t) \right\}. \quad (12) \end{aligned}$$

In the i^{th} term of the summation in Eq. (12), we change the variables of integration from $\underline{\underline{r}}'$ and $\underline{\underline{v}}'$

to

$$\left. \begin{aligned} \underline{r} &= \underline{R}_i(\underline{r}', \underline{v}', t) \\ \text{and} \\ \underline{v} &= \underline{R}_i(\underline{r}', \underline{v}', t) \end{aligned} \right\} \quad (13)$$

The Jacobian of this transformation is unity for each i . We now assume, for all $\underline{r}'$ and $\underline{v}'$ for which $f_i(\underline{r}', \underline{v}', 0)$ does not vanish, and for all t between t_1 and t_2 , that $\underline{r}$ as given by Eq. (13) lies within the volume V or on its boundary. This can be achieved by choosing the nonelectromagnetic potentials, U_i , appropriately. Let the inverse of Eqs. (13) be written as

$$\left. \begin{aligned} \underline{r}' &= \underline{G}_i(\underline{r}, \underline{v}, t) \\ \text{and} \\ \underline{v}' &= \underline{K}_i(\underline{r}, \underline{v}, t) \end{aligned} \right\} \quad (14)$$

and use the identity

$$f_i(\underline{r}, \underline{v}, t) = f_i[\underline{G}_i(\underline{r}, \underline{v}, t), \underline{K}_i(\underline{r}, \underline{v}, t), 0] \quad (15)$$

Then we can rewrite Eq. (12) as

$$\begin{aligned} \delta \varphi \int_{t_1}^{t_2} L dt &= \int_{t_1}^{t_2} dt \int_V d^3 \underline{r} \left\{ \left[- \sum_{i=1}^N \int d^3 \underline{v} q_i f_i(\underline{r}, \underline{v}, t) \right] \right. \\ &\quad \left. + \frac{1}{4\pi} \nabla \cdot \underline{D}(\underline{r}, t) - \rho_o(\underline{r}, t) \right\} \delta \varphi(\underline{r}, t) \quad (16) \end{aligned}$$

Here we have used the first of Eqs. (7) and have required

$$\begin{aligned} \int_V d^3 \underline{r} \nabla \cdot \underline{D}(\underline{r}, t) \delta \varphi(\underline{r}, t) \\ = \int_{\text{boundary of } V} dS \cdot \left[\delta \varphi(\underline{r}, t) \underline{D}(\underline{r}, t) \right] = 0. \quad (16a) \end{aligned}$$

To satisfy this requirement, we shall normally have to require either periodic boundary conditions on $\delta \varphi$ and the normal component of $\underline{D}$ or require $\delta \varphi = 0$ on the boundary of V . Since the variation in Eq. (16) must vanish for arbitrary $\delta \varphi$ that satisfies the boundary conditions on the boundary of V , the expression within the curly brackets of Eq. (16) must vanish, and we thus obtain the third of Eqs. (6).

To derive the last of Eqs. (6), we vary the

integral of the Lagrangian with respect to $\underline{A}$, with the result

$$\begin{aligned} \delta \underline{A} \int_{t_1}^{t_2} L dt &= \sum_{i=1}^N \int_{t_1}^{t_2} dt \int d^3 \underline{r}' d^3 \underline{v}' f_i(\underline{r}', \underline{v}', 0) \frac{1}{c} q_i \underline{R}_i \cdot \delta \underline{A}(\underline{R}_i, t) \\ &\quad + \int_{t_1}^{t_2} dt \int_V d^3 \underline{r} \left\{ - \frac{1}{c} \left[\nabla \cdot \underline{E}(\underline{r}, t) \right] \cdot \delta \left[\underline{A}(\underline{r}, t) \right] \right. \\ &\quad \left. - \left[\nabla \times \underline{B}(\underline{r}, t) \right] \cdot \delta \left[\underline{A}(\underline{r}, t) \right] + \frac{1}{c} \underline{j}_o(\underline{r}, t) \cdot \delta \underline{A}(\underline{r}, t) \right\}. \quad (17) \end{aligned}$$

We now transform the integrals in the summation in this expression in the same manner in which the corresponding integrals were transformed for the variation with respect to φ . Then the variation with respect to $\underline{A}$ can be written as

$$\begin{aligned} \delta \underline{A} \int_{t_1}^{t_2} L dt &= \int_{t_1}^{t_2} dt \int_V d^3 \underline{r} \left\{ \left[\sum_{i=1}^N \int d^3 \underline{v} \frac{1}{c} q_i \underline{v} f_i(\underline{r}, \underline{v}, t) \right] \right. \\ &\quad \left. + \frac{1}{4\pi c} \underline{D}(\underline{r}, t) - \frac{1}{4\pi} \nabla \times \underline{H}(\underline{r}, t) + \frac{1}{c} \underline{j}_o(\underline{r}, t) \right\} \cdot \delta \underline{A}(\underline{r}, t). \quad (18) \end{aligned}$$

Here we have used the second of Eqs. (7), and we have required that the component of $\delta \underline{A}$ along $\underline{D}$ vanish at times t_1 and t_2 . We have also required

$$\begin{aligned} \int_V d^3 \underline{r} \nabla \cdot \left[\delta \underline{A}(\underline{r}, t) \times \underline{H}(\underline{r}, t) \right] \\ = \int_{\text{boundary of } V} dS \cdot \left[\delta \underline{A}(\underline{r}, t) \times \underline{H}(\underline{r}, t) \right] = 0. \quad (18a) \end{aligned}$$

Normally, to satisfy this condition we shall either have to require periodic boundary conditions on the normal component of $\delta \underline{A} \times \underline{H}$, or require that the component of $\delta \underline{A}$ transverse to $\underline{H}$ vanish on the boundary of V . The vanishing of this variation for arbitrary $\delta \underline{A}$ that satisfies the conditions at times t_1 and t_2 and on the boundary of V requires that the expression within the curly brackets of Eq. (18) vanish, and this gives the last of Eqs. (6).

We have now shown that satisfying Hamilton's principle, Eq. (10), leads to the correct equations of motion for the system, provided that $\delta \underline{R}_k$ and the component of $\delta \underline{A}$ along $\underline{D}$ vanish at times t_1 and t_2 , provided that the boundary conditions expressed by Eqs. (16a) and (18a) are satisfied, and provided that the $\underline{r}$ given by Eq. (13) lies within the volume V or on its boundary for t between t_1 and t_2 and for all $\underline{r}'$ and $\underline{v}'$ for which $f_1(\underline{r}', \underline{v}', 0)$ does not vanish.

C. Initial and Boundary Conditions on the Electromagnetic Potentials

The boundary conditions on the electromagnetic potentials that were derived in the previous section are expressed in terms of the potentials by Eqs. (16a) and (18a). Normally these conditions are satisfied by requiring either that $\delta \varphi$ and the component of $\delta \underline{A}$ transverse to $\underline{H}$ vanish on the boundary of V , or that the normal component of $\delta \varphi \underline{D}$ and the normal component of $\delta \underline{A} \times \underline{H}$ satisfy periodic boundary conditions,* or some combination of these. The approximate representations of φ and $\underline{A}$ that we shall introduce later must be chosen to satisfy appropriate boundary conditions.

The initial conditions on $\underline{A}$ that were derived are that the component of $\delta \underline{A}$ along $\underline{D}$ vanish at times t_1 and t_2 . That this initial condition involves only one component of $\delta \underline{A}$ is inconvenient for the purpose of using Hamilton's principle to derive an approximate set of equations. However, because of the gauge invariance of the electromagnetic field, we also have considerable freedom to impose conditions on the component of $\delta \underline{A}$ transverse to $\underline{D}$ at times t_1 and t_2 . In particular, we can require that $\delta \underline{A}$, all components of it, satisfy $\delta \underline{A} = 0$ at times t_1 and t_2 . These are the initial conditions that we shall use in deriving the approximate equations.

To demonstrate the equivalence of these two sets of initial conditions, we first note that the electromagnetic potentials are only needed for computing the electric and magnetic fields. When the potentials are varied in the action integral, they

* If the potentials satisfy periodic boundary conditions, then so do their variations and the fields $\underline{E}$ and $\underline{B}$. If, in addition, the functions χ and ψ satisfy periodic boundary conditions in their explicit dependence on $\underline{r}$, then the fields $\underline{D}$ and $\underline{H}$ will also satisfy periodic boundary conditions.

only need be varied within a class of functions that satisfy the boundary and initial conditions that we have deduced and from which all allowable electric and magnetic fields can be derived. There are many such classes of functions, and they are related by gauge transformations.

Consider a $\delta \varphi(\underline{r}, t)$ and a $\delta \underline{A}(\underline{r}, t)$ such that $\underline{D}(\underline{r}, t_0) \cdot \delta \underline{A}(\underline{r}, t_0) = 0$, where t_0 can assume the two values t_1 and t_2 , and the component of $\delta \underline{A}(\underline{r}, t_0)$ perpendicular to $\underline{D}(\underline{r}, t_0)$ is allowed to be arbitrary. The corresponding variations of $\underline{E}(\underline{r}, t)$ and $\underline{B}(\underline{r}, t)$ are

$$\delta \underline{E}(\underline{r}, t) = -\delta \nabla \varphi(\underline{r}, t) - \frac{1}{c} \delta \frac{\partial \underline{A}(\underline{r}, t)}{\partial t}$$

$$= -\nabla \delta \varphi(\underline{r}, t) - \frac{1}{c} \frac{\partial}{\partial t} \delta \underline{A}(\underline{r}, t)$$

$$\delta \underline{B}(\underline{r}, t) = \delta \nabla \times \underline{A}(\underline{r}, t) = \nabla \times \delta \underline{A}(\underline{r}, t).$$

Since the electromagnetic field which interests us satisfies initial conditions that make it unique, the variations of the potentials are restricted by the requirement $\delta \underline{B}(\underline{r}, t_0) = 0$. Therefore, $\nabla \times \delta \underline{A}(\underline{r}, t_0)$ vanishes and $\delta \underline{A}(\underline{r}, t_0)$ is the gradient of a scalar function. We now make a gauge transformation to new variations of the potentials, denoting the new variations by primes. To ensure that the new variations can be used in Hamilton's principle, we require $\underline{D}(\underline{r}, t_0) \cdot [\delta \underline{A}(\underline{r}, t_0)]' = 0$.

$$[\delta \underline{A}(\underline{r}, t)]' = \delta \underline{A}(\underline{r}, t) + \nabla \eta(\underline{r}, t).$$

$$[\delta \varphi(\underline{r}, t)]' = \delta \varphi(\underline{r}, t) - \frac{1}{c} \frac{\partial \eta(\underline{r}, t)}{\partial t}.$$

The variations of $\underline{E}(\underline{r}, t)$ and $\underline{B}(\underline{r}, t)$ are left unchanged by this transformation. We can now make $[\delta \underline{A}(\underline{r}, t_0)]'$ vanish and specify $[\delta \varphi(\underline{r}, t_0)]'$ arbitrarily by choosing $\nabla \eta(\underline{r}, t_0)$ and $\partial \eta(\underline{r}, t)/\partial t|_{t=t_0}$ appropriately. In particular, we choose

$$\nabla \eta(\underline{r}, t_0) = -\delta \underline{A}(\underline{r}, t_0).$$

Thus, we have shown that we can, without loss of generality, vary the potentials in a gauge that allows

$$\delta \underline{A}(\underline{r}, t_0) = 0, \quad t_0 = t_1 \text{ or } t_2, \quad (19)$$

as initial conditions.

III. DERIVATION OF AN APPROXIMATE SYSTEM OF FIRST-ORDER EQUATIONS FROM HAMILTON'S PRINCIPLE

A. Choice of Representation

We must now decide in what form to represent the unknown functions, φ , A , and R_k , approximately. We choose to represent $\varphi(\underline{r}, t)$ and $A(\underline{r}, t)$ as linear combinations of finite numbers of specified, linearly independent basis functions of $\underline{r}$ with time-dependent coefficients, plus specified functions that satisfy the boundary conditions, and to represent the coordinates of $R_k(\underline{r}', \underline{v}', t)$ as linear combinations of finite numbers of specified, linearly independent basis functions of $\underline{r}'$ and $\underline{v}'$ with time-dependent coefficients. The representations of $\varphi(\underline{r}, t)$ and $A(\underline{r}, t)$ are

$$\left. \begin{aligned} \varphi(\underline{r}, t) &= \varphi_0(\underline{r}, t) + \sum_{i=1}^{M_0} \alpha_i(t) \Phi_i(\underline{r}) \\ A(\underline{r}, t) &= A_0(\underline{r}, t) + \sum_{j=1}^3 \hat{e}_j \sum_{i=1}^{M_j} \beta_{ji}(t) Q_{ji}(\underline{r}) \end{aligned} \right\} \quad (20)$$

The vectors $\hat{e}_j$ are a right-handed set of orthogonal unit vectors that may be the unit vectors of a curvilinear coordinate system:

$$\hat{e}_k = \hat{e}_i \times \hat{e}_j, \quad (ijk) \text{ cyclic.}$$

The functions $\varphi_0(\underline{r}, t)$ and $A_0(\underline{r}, t)$ are specified in advance and chosen to satisfy the boundary conditions, either exactly or in some suitably approximate way. The functions $\Phi_i(\underline{r})$ and $\hat{e}_j Q_{ji}(\underline{r})$ are specified and linearly independent. In addition, the functions $\Phi_i(\underline{r})$ and $Q_{ji}(\underline{r})$ satisfy homogeneous boundary conditions; that is, each of the functions vanishes on the boundary of V . The variations of φ and A are

$$\left. \begin{aligned} \delta\varphi(\underline{r}, t) &= \sum_{i=1}^{M_0} \delta\alpha_i(t) \Phi_i(\underline{r}) \\ \delta A(\underline{r}, t) &= \sum_{j=1}^3 \hat{e}_j \sum_{i=1}^{M_j} \delta\beta_{ji}(t) Q_{ji}(\underline{r}) \end{aligned} \right\} \quad (21)$$

*If φ and A are to satisfy periodic boundary conditions, then the Φ_i and Q_{ji} should satisfy periodic boundary conditions also, and the φ_0 and A_0 may be set equal to zero.

Because the Φ_i and Q_{ji} satisfy either homogeneous or periodic boundary conditions, the variations of Eq. (21) either vanish or are periodic on the boundary of V . Because the $\hat{e}_j Q_{ji}$ are linearly independent, the condition $\delta A(\underline{r}, t_0) = 0$ implies

$$\delta\beta_{ji}(t_0) = 0, \quad t_0 = t_1 \text{ or } t_2. \quad (21a)$$

We denote the coordinates of $R_k(\underline{r}', \underline{v}', t)$ by $x_{kj}(\underline{r}', \underline{v}', t)$, ($j = 1, 2, 3$). The representations of the x_{kj} are

$$x_{kj}(\underline{r}', \underline{v}', t) = x_{kj}^{(0)}(\underline{r}', \underline{v}', t) + \sum_{i=1}^{N_{kj}} \gamma_{kji}(t) x_{kji}(\underline{r}', \underline{v}'). \quad (22)$$

The functions $x_{kj}^{(0)}(\underline{r}', \underline{v}', t)$ are arbitrary and specified in advance; for example, they may be chosen to satisfy the initial conditions on the $x_{kji}(\underline{r}', \underline{v}', t)$. The set of $x_{kji}(\underline{r}', \underline{v}')$ for fixed k and j are specified in advance and linearly independent.

Three coordinate systems will be treated explicitly: cartesian, cylindrical, and toroidal.

Cartesian coordinates

$\hat{e}_1$, $\hat{e}_2$, and $\hat{e}_3$ are unit vectors in the directions of increasing x , y , and z , respectively; and x_{k1} , x_{k2} , and x_{k3} are the x , y , and z coordinates of R_k , respectively. R_k , its first two time derivatives, and its variation are:

$$\underline{R}_k(\underline{r}', \underline{v}', t) = \sum_{j=1}^3 \hat{e}_j x_{kj}(\underline{r}', \underline{v}', t), \quad (23a)$$

$$\dot{\underline{R}}_k(\underline{r}', \underline{v}', t) = \sum_{j=1}^3 \hat{e}_j \dot{x}_{kj}(\underline{r}', \underline{v}', t), \quad (23b)$$

$$\ddot{\underline{R}}_k(\underline{r}', \underline{v}', t) = \sum_{j=1}^3 \hat{e}_j \ddot{x}_{kj}(\underline{r}', \underline{v}', t), \quad (23c)$$

$$\begin{aligned} \delta \underline{R}_k(\underline{r}', \underline{v}', t) &= \sum_{j=1}^3 \hat{e}_j \delta x_{kj}(\underline{r}', \underline{v}', t) \\ &= \sum_{j=1}^3 \hat{e}_j \delta y_{kji}(t) x_{kji}(\underline{r}', \underline{v}'). \end{aligned} \quad (23d)$$

Because of the linear independence of the basis functions, the condition $\delta \underline{R}_k(\underline{r}', \underline{v}', t_0) = 0$ implies

$$\delta y_{kji}(t_0) = 0, \quad t_0 = t_1 \text{ or } t_2 \quad (24)$$

Cylindrical coordinates

$\hat{e}_1$, $\hat{e}_2$, and $\hat{e}_3$ are unit vectors in the directions of increasing r , θ , and z , respectively; and x_{k1} , x_{k2} , and x_{k3} are the r , θ , and z coordinates of $\underline{R}_k$, respectively. The nonzero derivatives of the unit vectors are

$$\frac{\partial \hat{e}_1}{\partial \theta} = \frac{\partial \hat{r}}{\partial \theta} = \hat{\theta} = \hat{e}_2,$$

$$\frac{\partial \hat{e}_2}{\partial \theta} = \frac{\partial \hat{\theta}}{\partial \theta} = -\hat{r} = -\hat{e}_1.$$

$\underline{R}_k$, its first two-time derivatives, and its variation are:

$$\begin{aligned} \underline{R}_k(\underline{r}', \underline{v}', t) &= \hat{e}_1 x_{k1}(\underline{r}', \underline{v}', t) \\ &+ \hat{e}_2 x_{k2}(\underline{r}', \underline{v}', t), \end{aligned} \quad (25a)$$

$$\begin{aligned} \dot{\underline{R}}_k(\underline{r}', \underline{v}', t) &= \hat{e}_1 \dot{x}_{k1}(\underline{r}', \underline{v}', t) \\ &+ \hat{e}_2 \dot{x}_{k1}(\underline{r}', \underline{v}', t) \dot{x}_{k2}(\underline{r}', \underline{v}', t) \\ &+ \hat{e}_3 \dot{x}_{k3}(\underline{r}', \underline{v}', t), \end{aligned} \quad (25b)$$

$$\begin{aligned} \ddot{\underline{R}}_k(\underline{r}', \underline{v}', t) &= \hat{e}_1 \left\{ \ddot{x}_{k1}(\underline{r}', \underline{v}', t) - x_{k1}(\underline{r}', \underline{v}', t) [\dot{x}_{k2}(\underline{r}', \underline{v}', t)]^2 \right\} \\ &+ \hat{e}_2 \left\{ \dot{x}_{k1}(\underline{r}', \underline{v}', t) \ddot{x}_{k2}(\underline{r}', \underline{v}', t) \right. \\ &\quad \left. + 2 \dot{x}_{k1}(\underline{r}', \underline{v}', t) \dot{x}_{k2}(\underline{r}', \underline{v}', t) \right\} \\ &+ \hat{e}_3 \ddot{x}_{k3}(\underline{r}', \underline{v}', t), \end{aligned} \quad (25c)$$

$$\begin{aligned} \delta \underline{R}_k(\underline{r}', \underline{v}', t) &= \hat{e}_1 \delta x_{k1}(\underline{r}', \underline{v}', t) \\ &+ \hat{e}_2 x_{k1}(\underline{r}', \underline{v}', t) \delta x_{k2}(\underline{r}', \underline{v}', t) + \hat{e}_3 \delta x_{k3}(\underline{r}', \underline{v}', t) \\ &= \hat{e}_1 \sum_{i=1}^{N_{k1}} \delta y_{k1i}(t) x_{k1i}(\underline{r}', \underline{v}') \\ &\quad + \hat{e}_2 \left[x_{k1}^{(u)}(\underline{r}', \underline{v}', t) + \sum_{i=1}^{N_{k1}} y_{k1i}(t) \dot{x}_{k1i}(\underline{r}', \underline{v}') \right] \\ &\quad \cdot \left[\sum_{n=1}^{N_{k2}} \delta y_{k2n}(t) \dot{x}_{k2n}(\underline{r}', \underline{v}') \right] \\ &\quad + \hat{e}_3 \sum_{i=1}^{N_{k3}} \delta y_{k3i}(t) x_{k3i}(\underline{r}', \underline{v}'). \end{aligned} \quad (25d)$$

Because of the linear independence of the basis functions, the condition $\delta \underline{R}_k(\underline{r}', \underline{v}', t_0) = 0$ implies

$$\delta y_{kji}(t_0) = 0, \quad t_0 = t_1 \text{ or } t_2. \quad (24)$$

Toroidal coordinates

ϕ increases counterclockwise looking along $\hat{k}$. z is defined by $z = \rho_0 \phi$. $\hat{e}_1$, $\hat{e}_2$, and $\hat{e}_3$ are unit vectors in the directions of increasing r , θ , and z , respectively; and χ_{k1} , χ_{k2} , and χ_{k3} are the r , θ , and z coordinates of R_k , respectively. The nonzero derivatives of the unit vectors are

$$\frac{\partial \hat{e}_1}{\partial \theta} = \frac{\partial \hat{r}}{\partial \theta} = \hat{\theta} = \hat{e}_2,$$

$$\frac{\partial \hat{e}_1}{\partial \phi} = \frac{\partial \hat{r}}{\partial \phi} = \hat{\phi} \cos \theta = \hat{e}_3 \cos \theta,$$

$$\frac{\partial \hat{e}_2}{\partial \theta} = \frac{\partial \hat{\theta}}{\partial \theta} = -\hat{r} = -\hat{e}_1,$$

$$\frac{\partial \hat{e}_2}{\partial \phi} = \frac{\partial \hat{\theta}}{\partial \phi} = -\hat{\phi} \sin \theta = -\hat{e}_3 \sin \theta,$$

$$\frac{\partial \hat{e}_3}{\partial \phi} = \frac{\partial \hat{\phi}}{\partial \phi} = \hat{\phi} \times \hat{k}$$

$$= -\hat{r} \cos \theta + \hat{\theta} \sin \theta = -\hat{e}_1 \cos \theta + \hat{e}_2 \sin \theta.$$

R_k , its first two time derivatives, and its variation are:

$$\begin{aligned} R_k(r', v', t) &= \hat{e}_1 \left\{ \rho_0 \cos \chi_{k2}(r', v', t) + \chi_{k1}(r', v', t) \right\} \\ &\quad - \hat{e}_2 \rho_0 \sin \chi_{k2}(r', v', t), \end{aligned} \quad (26a)$$

$$\begin{aligned} \dot{R}_k(r', v', t) &= \hat{e}_1 \dot{\chi}_{k1}(r', v', t) \\ &\quad + \hat{e}_2 \chi_{k1}(r', v', t) \dot{\chi}_{k2}(r', v', t) \\ &\quad + \hat{e}_3 \left\{ 1 + \frac{1}{\rho_0} \chi_{k1}(r', v', t) \cos \chi_{k2}(r', v', t) \right\} \\ &\quad \cdot \dot{\chi}_{k3}(r', v', t), \end{aligned} \quad (26b)$$

$$\begin{aligned} \ddot{R}_k(r', v', t) &= \hat{e}_1 \left\{ \ddot{\chi}_{k1}(r', v', t) - \chi_{k1}(r', v', t) \dot{\chi}_{k2}^2(r', v', t) \right. \\ &\quad - \frac{1}{\rho_0} \left[1 + \frac{1}{\rho_0} \chi_{k1}(r', v', t) \cos \chi_{k2}(r', v', t) \right] \\ &\quad \cdot \dot{\chi}_{k3}^2(r', v', t) \cos \chi_{k2}(r', v', t) \Big\} \\ &\quad + \hat{e}_2 \left\{ \ddot{\chi}_{k1}(r', v', t) \dot{\chi}_{k2}(r', v', t) \right. \\ &\quad + 2 \dot{\chi}_{k1}(r', v', t) \dot{\chi}_{k2}(r', v', t) \\ &\quad + \frac{1}{\rho_0} \left[1 + \frac{1}{\rho_0} \chi_{k1}(r', v', t) \cos \chi_{k2}(r', v', t) \right] \\ &\quad \cdot \dot{\chi}_{k3}^2(r', v', t) \sin \chi_{k2}(r', v', t) \Big\} \\ &\quad + \hat{e}_3 \left\{ \left[1 + \frac{1}{\rho_0} \chi_{k1}(r', v', t) \cos \chi_{k2}(r', v', t) \right] \right. \\ &\quad \cdot \ddot{\chi}_{k3}(r', v', t) \\ &\quad + 2 \left[\frac{1}{\rho_0} \dot{\chi}_{k1}(r', v', t) \cos \chi_{k2}(r', v', t) \right. \\ &\quad - \frac{1}{\rho_0} \chi_{k1}(r', v', t) \dot{\chi}_{k2}(r', v', t) \sin \chi_{k2}(r', v', t) \Big] \\ &\quad \cdot \dot{\chi}_{k3}(r', v', t) \Big\}, \end{aligned} \quad (26c)$$

$$\begin{aligned} \delta R_k(r', v', t) &= \hat{e}_1 \delta \chi_{k1}(r', v', t) \\ &\quad + \hat{e}_2 \left\{ \chi_{k1}(r', v', t) \right\} \delta \chi_{k2}(r', v', t) \\ &\quad + \hat{e}_3 \left\{ 1 + \frac{1}{\rho_0} \chi_{k1}(r', v', t) \cos \chi_{k2}(r', v', t) \right\} \\ &\quad \cdot \delta \chi_{k3}(r', v', t). \end{aligned} \quad (26d)$$

As before, because of the linear independence of the basis functions, the condition $\delta R_k(r', v', t_0) = 0$ implies

$$\delta \gamma_{kji}(t_0) = 0, \quad t_0 = t_1 \text{ or } t_2. \quad (24)$$

B. Initial Conditions for the γ_{kji}

The initial conditions for the $\gamma_{kji}(t)$ must be chosen in the way that satisfies the initial conditions on the $R_k(r', v', t)$, Eqs. (5). A convenient way of doing this is to choose functions $\chi_{kj}^{(0)}(r', v', t)$ that satisfy the initial conditions on the $\chi_{kj}(r', v', t)$. Then the initial conditions for the $\gamma_{kji}(t)$ are

$$\gamma_{kji}(0) = 0 \quad (27)$$

and

$$\gamma_{kji}(0) = 0. \quad (28)$$

C. Application of Hamilton's Principle

In the remainder of this report we frequently shall not indicate the arguments of the basis functions explicitly.

We are now in a position to apply Hamilton's principle. Since the approximate representations of the unknown functions -- φ , $\underline{A}$, and $\underline{R}_k$ -- have been so chosen that they and their variations satisfy the same initial and boundary conditions that were assumed in deriving the exact equations, therefore we can use results from Section II directly.

In this section we shall describe how Eqs. (11), (12), and (17) are used to derive equations for γ_{kji} , α_i , and β_{ji} ; and we shall discuss some aspects of the equations. Because of the generality of the presentation up to this point and the complexity of the equations, we shall not write the equations explicitly for the general case in a general curvilinear coordinate system. In Section IV the equations will be written explicitly for a simple special case.

Equations for the $\gamma_{kji}(t)$ are obtained by setting the variation of the integral of the Lagrangian with respect to $\underline{R}_k$, given by Eq. (11), equal to zero:

$$\begin{aligned} 0 = & \int_{t_1}^{t_2} dt \int d^3r' d^3v' f_k(r', v', 0) \left\{ m_{kk} \ddot{\underline{R}}_k - \frac{d}{dt} \nabla_k U_k(\underline{R}_k, \dot{\underline{R}}_k, t) \right. \\ & + \nabla_k U_k(\underline{R}_k, \dot{\underline{R}}_k, t) + q_k \left[\nabla_k \varphi(\underline{R}_k, t) + \frac{1}{c} \dot{\underline{A}}(\underline{R}_k, t) \right] \\ & \left. - \frac{1}{c} q_k \dot{\underline{R}}_k \times \left[\nabla_{\underline{R}_k} \times \underline{A}(\underline{R}_k, t) \right] \right\} \cdot \delta \underline{R}_k. \quad (29) \end{aligned}$$

The $\delta \underline{R}_k$ in this equation is a linear combination of the $\delta \gamma_{kji}$. Equation (29) is an integral over t whose integrand is a definite integral over $\underline{r}'$ and $\underline{v}'$. Since the $\delta \gamma_{kji}$ are independent of one another, the coefficient of each $\delta \gamma_{kji}$ in the integrand must vanish. The equations obtained by setting each coefficient equal to zero are a set of second-order differential equations for the γ_{kji} that are

coupled to the α_i and β_{ji} . The equations are linear in the $\ddot{\gamma}_{kji}$ because the expression

$$m_{kk} \ddot{\underline{R}}_k - \frac{d}{dt} \nabla_k U_k(\underline{R}_k, \dot{\underline{R}}_k, t)$$

is linear in $\underline{R}_k$.

Equations for the $\alpha_i(t)$ and $\beta_{ji}(t)$ are obtained by setting the variations of the integral of the Lagrangian with respect to φ , given by Eq. (12), and with respect to $\underline{A}$, given by Eq. (17), equal to zero:

$$\begin{aligned} 0 = & \int_{t_1}^{t_2} dt \left\{ \int_V d^3r \left[\frac{1}{4\pi} D(\underline{r}, t) \cdot \delta(\nabla \varphi(\underline{r}, t)) \right. \right. \\ & \left. \left. + \rho_0(\underline{r}, t) \delta \varphi(\underline{r}, t) \right] \right. \\ & \left. + \sum_{i=1}^N \int d^3r' d^3v' f_i(r', v', 0) q_i \delta \varphi(\underline{R}_i, t) \right\}, \quad (30) \end{aligned}$$

$$\begin{aligned} 0 = & \int_{t_1}^{t_2} dt \left\{ \int_V d^3r \left[-\frac{1}{4\pi} H(\underline{r}, t) \cdot \delta(\nabla \times \underline{A}(\underline{r}, t)) \right. \right. \\ & \left. \left. + \frac{1}{c} \underline{j}_0(\underline{r}, t) \cdot \delta \underline{A}(\underline{r}, t) + \frac{1}{4\pi c} \dot{\underline{D}}(\underline{r}, t) \cdot \delta \underline{A}(\underline{r}, t) \right] \right. \\ & \left. + \sum_{i=1}^N \int d^3r' d^3v' f_i(r', v', 0) \frac{1}{c} q_i \dot{\underline{R}}_i \cdot \delta \underline{A}(\underline{R}_i, t) \right\}. \quad (31) \end{aligned}$$

As before, the vectors $\underline{D}(\underline{r}, t)$ and $\underline{H}(\underline{r}, t)$ are to be representable as in Eqs. (7). The $\delta \varphi$ and $\delta \underline{A}$ in Eqs. (30) and (31) are linear combinations of the $\delta \alpha_i$ and $\delta \beta_{ji}$. Each equation is an integral over t whose integrand is a sum of definite integrals over $\underline{r}$ and over $\underline{r}'$ and $\underline{v}'$. Since the $\delta \alpha_i$ and $\delta \beta_{ji}$ are independent of one another, the coefficient of each $\delta \alpha_i$ in the integrand of Eq. (30) must vanish, and the coefficient of each $\delta \beta_{ji}$ in the integrand of Eq. (31) must also vanish. The equations obtained by setting each coefficient equal to zero are of second order for the β_{ji} and first order for the α_i . The equations are linear in the $\ddot{\beta}_{ji}$ and $\dot{\alpha}_i$ because of Eqs. (7) and (8).

The approximate equations to be solved are those obtained from Eqs. (29)-(31) in the manner just described. It may be convenient to reformulate the approximate equations somewhat by defining new variables in terms of which we have a system of first-order equations. The new variables are

$$\omega_{ji}(t) = \dot{\beta}_{ji}(t)$$

and

$$\eta_{kji}(t) = \dot{\gamma}_{kji}(t).$$

(32)

The equations obtained from Eq. (30) are first solved algebraically for the α_1 in terms of the ω_{ji} and γ_{kji} . The remaining equations (including Eqs. (32)) are then a system of first-order equations for the η_{kji} , γ_{kji} , ω_{ji} , and β_{ji} .

The approximate equations obtained from Eqs. (29)-(31) could also be obtained from the exact differential equations by taking weighted inner products of the exact differential equations with the basis functions, using Liouville's theorem to replace $f_i(\underline{r}, \underline{v}, t)$ by $f_i(\underline{r}', \underline{v}', 0)$, the inverse of what was done in deriving Eqs. (16) and (18), and performing appropriate partial integrations. The inner products with Newton's law would have to be taken with $f_i(\underline{r}', \underline{v}', 0)$ times the coefficients of the $\delta\gamma_{kji}$ in δR_k as weight functions, and those with Maxwell's equations taken with unit weight function. Hamilton's principle has specified the weight functions to be used.

D. Choice of Basis Functions

To solve the equations for the time-dependent coefficients, the definite integrals over $\underline{r}$ and over $\underline{r}'$ and $\underline{v}'$ must be evaluated. In general, these integrals must be evaluated numerically at each time step during numerical integration of the equations for the time-dependent coefficients. However, there are cases in which it is possible to perform the integrals analytically at the outset. The basic obstacle that prevents performing the integrals analytically is that Eqs. (29)-(31) involve unknown functions of unknown functions. It is not generally possible to perform the integrals analytically for arbitrary values of the time-dependent coefficients. If, however, the functions U_k and the basis functions for ϕ and A are polynomial functions of their arguments, and if $\underline{D}$ and $\underline{H}$ are polynomial functions of $\underline{E}$ and $\underline{B}$, then all of the time-dependent coefficients in the integrands can be separated out explicitly, so that the integrands are sums of products of functions of time with functions of the variables of integration. If, in addition, the $f_k(\underline{r}', \underline{v}', 0)$ and the other functions of the variables of integration are chosen appropriately, then the integrals can be

performed analytically at the outset.

If polynomial functions are used, we are effectively prevented from using curvilinear coordinates because of the requirement that functions of angle variables be periodic. Similarly, periodic boundary conditions are generally not allowable if polynomial functions are used. It should also be noted that use of polynomial functions can lead to numerical difficulties as a result of the occurrence of large powers.

For cartesian coordinates, but usually not for curvilinear coordinates, it is possible to simplify the equations for the time-dependent coefficients by choosing the basis functions to satisfy certain orthogonality relations.

IV. A SIMPLE ONE-DIMENSIONAL EXAMPLE

A. The Basic Equations

We consider a one-dimensional, single-species plasma in the presence of a static, uniform, neutralizing background charge density. We denote the one spatial variable by x , and impose periodic boundary conditions at $x = 0$ and $x = L$. In addition, we restrict the electromagnetic field to be describable in terms of a scalar potential only. The equations for the time-dependent coefficients are obtained from Eqs. (29) and (30), and the representations of the unknown functions are given by Eqs. (20), (22), and (23). Since there are only one species and one spatial variable, we shall omit subscripts that distinguish the species and coordinates.

We denote the charge and mass of the particles by q and m , respectively. The uniform charge density is given by

$$\rho_0(x, t) = \rho = -\frac{q}{L} \int dx' dv' f(x', v', 0) = \text{constant}. \quad (33)$$

The vectors $\underline{D}$ and $\underline{H}$ are given by $\underline{D} = \underline{E}$, and $\underline{H} = \underline{B}$. The representations of the unknown functions are given by

$$\phi(x, t) = \sum_{i=1}^{M_0} \alpha_i(t) \Phi_i(x), \quad (34)$$

$$R(x', v', t) = \hat{e} \chi(x', v', t), \quad (35)$$

$$\chi(x', v', t) = x' + v't + \sum_{i=1}^N \gamma_i(t) X_i(x', v'). \quad (36)$$

The functions $\Phi_i(x)$ are to satisfy periodic boundary

conditions at $x = 0$ and $x = L$. The periodic nature of the system and the initial conditions on $\chi(x', v', t)$ require that $\chi(x', v', t)$ be represented as

$$\chi(x', v', t) = x' + v't + \sum_{i=1}^N \gamma_i(t) X_i(x', v'), \quad (37)$$

where the functions $X_i(x', v')$ satisfy periodic boundary conditions in x' at $x' = 0$ and $x' = L$, and where

$$\gamma_i(0) = \dot{\gamma}_i(0) = 0. \quad (38)$$

Equations (29) and (30) yield

$$\begin{aligned} 0 &= \int_{t_1}^{t_2} dt \int_0^L dx' \int dv' f(x', v', 0) \left\{ \sum_{i=1}^N \ddot{\gamma}_i(t) X_i(x', v') \right. \\ &+ q \sum_{i=1}^{M_0} \alpha_i(t) \Phi'_i[\chi(x', v', t)] \left. \right\} \sum_{j=1}^N \delta \gamma_j(t) X_j(x', v'), \\ 0 &= \int_{t_1}^{t_2} dt \left\{ \int_0^L dx \left[-\frac{1}{4\pi} \sum_{i=1}^{M_0} \alpha_i(t) \Phi'_i(x) \sum_{j=1}^{M_0} \delta \alpha_j(t) \Phi'_j(x) \right. \right. \\ &\quad \left. \left. + \rho \sum_{j=1}^{M_0} \delta \alpha_j(t) \Phi_j(x) \right] \right. \\ &\quad \left. + \int_0^L dx' \int dv' f(x', v', 0) q \sum_{j=1}^{M_0} \delta \alpha_j(t) \Phi_j[\chi(x', v', t)] \right\}. \end{aligned}$$

The primed functions are defined by

$$\Phi'_i(x) = \frac{d\Phi_i}{dx}.$$

Therefore, the equations for the $\alpha_i(t)$ and $\gamma_i(t)$ are

$$\begin{aligned} m \sum_{i=1}^N \ddot{\gamma}_i(t) \int_0^L dx' \int dv' f(x', v', 0) X_i(x', v') X_j(x', v') \\ = -q \sum_{i=1}^{M_0} \alpha_i(t) \int_0^L dx' \int dv' f(x', v', 0) \Phi'_i[\chi(x', v', t)] X_j(x', v'), \\ (j = 1, \dots, N) \quad (39) \end{aligned}$$

$$\frac{1}{4\pi} \sum_{i=1}^{M_0} \alpha_i(t) \int_0^L dx \Phi'_i(x) \Phi'_j(x) = \rho \int_0^L dx \Phi_j(x)$$

$$+ q \int_0^L dx' \int dv' f(x', v', 0) \Phi_j[\chi(x', v', t)]. \quad (40)$$

The set of equations represented by Eq. (40) can be solved for the $\alpha_i(t)$ in terms of the $\gamma_i(t)$, and then the expressions for the $\alpha_i(t)$ can be substituted into Eq. (39). This can be simplified considerably by choosing the Φ'_i to be orthogonal, as will be the case if the Φ_i are sines and cosines. We do so choose, and take the normalization such that

$$\frac{1}{4\pi} \int_0^L dx \Phi'_i(x) \Phi'_j(x) = \delta_{ij}. \quad (41)$$

Then

$$\begin{aligned} \alpha_i(t) &= \rho \int_0^L dx \Phi_i(x) \\ &+ q \int_0^L dx' \int dv' f(x', v', 0) \Phi_i[\chi(x', v', t)]. \quad (42) \end{aligned}$$

The equations represented by Eq. (39) are of the form

$$\sum_{i=1}^N C_{ji} \ddot{\gamma}_i = f_j(\{\gamma_k\}, t),$$

where the matrix elements C_{ji} are constants and $\{\gamma_k\}$ denotes the set of all γ_k . Therefore, they may be written as

$$\ddot{\gamma}_i = \sum_{j=1}^N (C^{-1})_{ij} f_j(\{\gamma_k\}, t),$$

which is probably a more convenient form for numerical work. The equations can be made first-order by introducing

$$\eta_i(t) = \dot{\gamma}_i(t).$$

In any event, the equations to be solved are those represented by Eq. (39) with $\alpha_i(t)$ defined by Eq. (42) and $\chi(x', v', t)$ defined by Eqs. (37)-(38).

The basis functions $X_i(x', v')$ and $\Phi_j(x)$ are still to be chosen subject to the boundary and orthogonality conditions that have been discussed.

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