Dynamics of a local algorithm for simulating Coulomb interactions

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Charged systems interacting via Coulomb forces can be efficiently simulated by introducing a local, diffusing degree of freedom for the electric field. This paper formulates the continuum electrodynamic equations corresponding to the algorithm and studies the spectrum of fluctuations when these equations are coupled to mobile charges. I compare the calculations with simulations of a charged lattice gas, and study the dynamics of charge and density fluctuations. The algorithm can be understood as a realization of a mechanical model of the ether. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1487821]

I. INTRODUCTION

Molecular dynamic simulation of charged condensed matter systems is slow and difficult.[1] In standard methods, such as optimized Ewald summation,[2,3] fast multipole methods[4,5] or the fast Fourier transform,[6] extensive and time consuming bookkeeping is needed because of the range of the Coulomb interaction. This bookkeeping often scales badly when implemented on modern multiprocessor machines which are used in the simulation of the largest systems. Naive Monte-Carlo methods are particularly inefficient since the motion of a single particle in an N particle simulation requires the recalculation of the Coulomb interaction with all other particles, leading to a complexity in $O(N)$ for an update in the position of a single particle.

Recently,[7] a *local algorithm* with complexity scaling as $O(1)$ per update was introduced for the Monte-Carlo simulation of charged particles. In this algorithm an auxiliary electric field $\mathbf{E}$ is coupled to the charge density. The dynamics of $\mathbf{E}$ are chosen so that the equilibrium distribution is determined by the Coulomb interaction. Due to the locality of the algorithm the method is trivial to implement on multiprocessor machines. In this paper we study the dynamics of the algorithm in order to understand the relaxation processes and time scales involved in a typical simulation. Simulations are performed on a model of a charged lattice gas to demonstrate the diffusive propagation of charge and density fluctuations.

The algorithm is based on implementing Gauss' law

$$\operatorname{div}\mathbf{E}=\rho/\epsilon_0, \tag{1}$$

in the equivalent integral form

$$\int \mathbf{E}.d\mathbf{S}=q/\epsilon_0, \tag{2}$$

as an exact dynamic constraint on the Monte-Carlo algorithm. Here ρ is the charge density and ϵ_0 the dielectric constant and q the charge enclosed by the surface of integration in Eq. (2).

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The system is discretized by placing charged particles on the vertices of a cubic lattice, $\{i\}$. The electric field $E_{i,j}$ is associated with the links $\{i,j\}$ of the lattice. The simulation starts with Gauss' law satisfied as an initial condition. There are two possible Monte-Carlo moves: First, Fig. 1, we displace a charge, e, situated on the leftmost lattice site, 1, to the rightmost site, 2. The discretized constraint is

$$\sum_j E_{i,j}=e_i/\epsilon_0, \tag{3}$$

with e_i the charge at the site i. The sum in Eq. (3) corresponds to the total electric flux leaving the site i. The constraint is again satisfied if the field associated with the connecting link is updated according to the rule $E_{1,2}\rightarrow E_{1,2}-e/\epsilon_0$. Second, we update the field configurations, Fig. 2, by modifying the four field values of a single plaquette by a pure rotation; $E_{1,2}$ and $E_{4,1}$ increase by an increment Δ whereas $E_{4,3}$ and $E_{3,2}$ decrease by Δ so that at each vertex the sum of the entering and leaving fields is unchanged. The basic *dynamic* degree of freedom in the second update is a circulation or rotation, $\mathbf{\Theta}$, associated with each plaquette of the network.

In the first section of the paper we formulate the continuum limit of the evolution equations and show that they lead to diffusive evolution of the electric field. We then couple the electric field to a mobile gas of charged particles and compare the solutions of the coupled plasma equations to simulations. Finally we show that the equations are closely related to the Maxwell electromagnetic theory.

II. DIFFUSIVE ELECTRODYNAMICS

A. Fundamental equations

We start with a simple example to motivate our derivation of the effective large scale equations obeyed by the electric field: a single particle diffusing in a harmonic potential with energy $\mathcal{U}=Kx^2/2$. The equation of motion is found by taking the derivative of the energy with respect to the dynamic coordinate x and then balancing the resulting force against a relaxation process linear in the velocity,

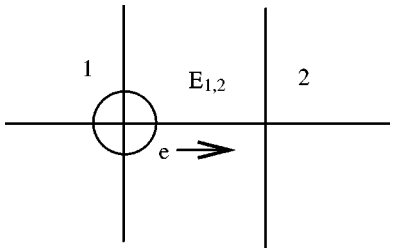

FIG. 1. Motion of a charge e from 1 to 2 is associated with a modification of the field on the connecting link: $E_{1,2}\rightarrow E_{1,2}-e/\epsilon_0$.

$$\xi\frac{dx}{dt}=-Kx+f(t), \tag{4}$$

where $f(t)$ is an external forcing term. ξ, the inverse mobility, sets the characteristic time scale of the relaxation of x and is a function of the step size of the Monte-Carlo trial moves. A first order (in time) algorithm, such as Monte-Carlo, for the simulation of a particle in such a potential (performed near equilibrium with small step sizes) is essentially a discretized realization of this stochastic differential equation. The Langevin description is completed by specifying f, so as to obey the fluctuation dissipation theorem.

We now turn to the equations for the electric field. First we examine the field in the absence of current then we shall find the coupling of the field to external sources. The discretized energy of the electric field is given by

$$\mathcal{U}=\frac{\epsilon_0}{2}\sum_{\text{links}}E_{i,j}^2. \tag{5}$$

The basic variables in the dynamics of the field are, however, not **E** but rather the rotational degrees of freedom which are updated independently at each time step. The conjugate force acting on this variable is a torque. We define on each plaquette in the $\{x,y\}$ plane the angular variable Θ^z. We group the angle corresponding to the three possible plaquette orientations into a vector $\mathbf{\Theta}$. The physical field **E** is sensitive to derivatives of $\mathbf{\Theta}$: Studying Fig. 2, one sees that $E_{1,2}$ is given by the x variation of the z component of $\mathbf{\Theta}$. This we recognize as part of the curl operator acting on the field $\mathbf{\Theta}$. The complete relation between a local variation in **E** and a local variation in $\mathbf{\Theta}$ is thus

$$\delta\mathbf{E}=\text{curl}\ \ \delta\mathbf{\Theta}, \tag{6}$$

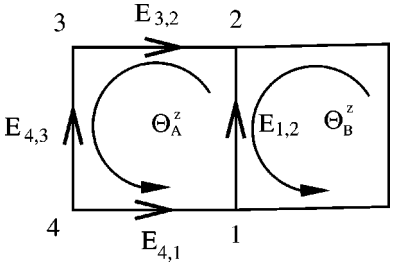

FIG. 2. Modification of the angle Θ_A^z leads to modified values of the field between on the links {1,2}, {3,2}, {4,3}, {4,1}. The field in the y direction associated with the link $E_{1,2}$ is given by the difference of the angles associated with the two plaquettes, Θ_A^z and Θ_B^z, which are aligned in the x direction.

where in the discretized model derivatives are to be understood as finite differences with **E** living on links and $\mathbf{\Theta}$ on plaquettes.

Modification of the circulation Θ_A^z in Fig. 2 by Δ gives rise to a new contribution to the energy of the plaquette:

$$\overline{\mathcal{U}}=\frac{\epsilon_0}{2}((E_{4,1}+\Delta)^2+(E_{1,2}+\Delta)^2+(E_{4,3}-\Delta)^2 +(E_{3,2}-\Delta)^2). \tag{7}$$

Taking the derivative with respect to Δ we find a torque, **C**, acting on the circulatory degree of freedom which is a discretized version of the curl of the field:

$$C_z=-\frac{\partial\overline{\mathcal{U}}}{\partial\Delta}=-\epsilon_0((E_{4,1}-E_{3,2})+(E_{1,2}-E_{4,3})), \tag{8}$$

$$=-\epsilon_0\left(\frac{\partial E^y}{\partial x}-\frac{\partial E^x}{\partial y}\right), \tag{9}$$

$$=-\epsilon_0\hat{\mathbf{k}}\cdot\text{curl}\ \ \mathbf{E}. \tag{10}$$

Again the three components of the torque live on the plaquettes together with the angle $\mathbf{\Theta}$. By analogy with Eq. (4), the evolution equation for the angle $\mathbf{\Theta}$ is

$$\xi\frac{d\mathbf{\Theta}}{dt}=\mathbf{C}=-\epsilon_0\ \ \text{curl}\ \ \mathbf{E}, \tag{11}$$

linking a velocity to the conjugate force. Eventually a stochastic force should also be added into this equation but we shall not need it in what follows.

Consider now the evolution of the field in the presence of a current. Take a network in which charges are present at *every* vertex and displace every charge to the right as in Fig. 1. Then every bond in the x direction is modified by $-e/\epsilon_0$ where e is the charge displaced even though the local charge density is unchanged. If we displace the charges at a constant rate we have the evolution of the field due to the source as

$$\frac{\partial\mathbf{E}_{\text{source}}}{\partial t}=-\mathbf{J}/\epsilon_0. \tag{12}$$

Combining Eqs. (6) and (12) we find

$$\frac{\partial\mathbf{E}}{\partial t}=-\mathbf{J}/\epsilon_0+\text{curl}\frac{\partial\mathbf{\Theta}}{\partial t}. \tag{13}$$

This equation is clearly analogous to the Maxwell equation,

$$\epsilon_0\frac{\partial\mathbf{E}}{\partial t}=-\mathbf{J}+\text{curl}\ \ \mathbf{H}, \tag{14}$$

if we write that $\mathbf{H}=\epsilon_0(\partial\mathbf{\Theta}/\partial t)$. We shall see later that **H** is indeed closely related to the magnetic degrees of freedom of classical electrodynamics. From Eqs. (10), (11), (13),

$$\frac{\partial\mathbf{E}}{\partial t}=(\epsilon_0\nabla^2\mathbf{E}-\text{grad}\,\rho)/\xi-\mathbf{J}/\epsilon_0, \tag{15}$$

where we have used the standard identity $(\text{curl}\,\mathbf{E})=(\text{grad div}\,\mathbf{E}-\nabla^2\mathbf{E})$ and Gauss' law. Equation (15) is the main result of this section giving a diffusive propagation law of the electric field in the absence of external charges and currents.

In the static limit both the current and the time derivative of Eq. (15) vanish. We find the same equation for the electric field,

$$\nabla^2 \mathbf{E} = \text{grad}\,\frac{\rho}{\epsilon_0}, \tag{16}$$

as is found by applying the operator $(-\text{grad})$ to the Poisson equation in conventional electrostatics. When we take the divergence of Eq. (15) we discover that

$$\left(\frac{\partial}{\partial t} - \frac{\epsilon_0}{\xi}\nabla^2\right)(\text{div}\,\mathbf{E} - \rho/\epsilon_0) = 0. \tag{17}$$

Again we see that Gauss' law is implemented in the method as an initial condition. Note that for this to be true we require that the Langevin noise associated with Eq. (15) does not in itself destroy the conservation law. It is thus the curl of some vector field.[8]

B. Relation to potentials

In our earlier paper[7] we showed that the electric field could be calculated from a scalar potential ϕ and a vector potential $\mathbf{Q}$ with the relationship

$$\mathbf{E} = -\text{grad}\,\phi + \text{curl}\;\mathbf{Q}. \tag{18}$$

In Fourier space we can write this equation as

$$\mathbf{E}(\mathbf{k}) = -i\mathbf{k}\phi + i\mathbf{k}\times\mathbf{Q}. \tag{19}$$

The second term of this expression is perpendicular to $\mathbf{k}$ so that there are two transverse degrees of freedom in the $\mathbf{Q}$ field, corresponding to two independent polarization states; the longitudinal component of $\mathbf{Q}$ is projected out and does not contribute to the electric field. We can consider that the field is due to a static longitudinal potential plus transverse photons.

If we take the time derivative of Eq. (18) we can compare with Eq. (13). The term curl $\dot{\mathbf{\Theta}}$ is purely transverse, whereas $-\mathbf{J}$ contains both longitudinal and transverse components. Thus we conclude that

$$\text{curl}\;\;\dot{\mathbf{Q}} = \text{curl}\;\;\dot{\mathbf{\Theta}} - \mathbf{J}_t/\epsilon_0 \tag{20}$$

and

$$\text{grad}\,\dot{\phi} = \mathbf{J}_l/\epsilon_0\,, \tag{21}$$

where $\mathbf{J}_t$ and $\mathbf{J}_l$ are the transverse and longitudinal components of the current. In general these are *nonlocal* relationships since the projection involves a passage via Fourier components. Such nonlocal relationships between potential and field are normal in the Coulomb gauge.[9]

C. Phenomenological dynamics of a two component plasma

In this section we couple the diffusive evolution equation for the electric field, Eq. (15), to the equations describing a two component plasma and study the relaxation phenomena and time scales that are to be expected when using the algorithm to simulate dense charged systems.

The equations of conservation and linear response give the following equations for the charge degrees of freedom:

$$\begin{aligned}
&\frac{\partial c^+}{\partial t} = -\,\text{div}\,\mathbf{J}^+,\\
&\frac{\partial c^-}{\partial t} = -\,\text{div}\,\mathbf{J}^-,\\
&\mathbf{J}^+ = -D\,\text{grad}\,c^+ + e\mu c^+\mathbf{E},\\
&\mathbf{J}^- = -D\,\text{grad}\,c^- - e\mu c^-\mathbf{E},
\end{aligned} \tag{22}$$

where c^+ and c^- are the number densities of the positive and negative charges, $\pm e$. $\mathbf{J}^{\pm}$ are the number current density. From these equations we find the equations obeyed by the total density c and the charge density ρ. We note that the diffusion coefficient D and the mobility, μ, are linked by the Einstein relation $D = k_B T\mu$.

Taking the sum and difference of the equations (22), we find

$$\begin{aligned}
&\frac{\partial c}{\partial t} = D\nabla^2 c,\\
&\frac{\partial \rho}{\partial t} = -\,\text{div}\,\mathbf{J}\\
&\mathbf{J} = e^2\mu c_0\mathbf{E} - D\,\text{grad}\,\rho - e^2 c_0\mu\,\text{grad}\,\phi_e(t),
\end{aligned} \tag{23}$$

where we have linearized the equations about a mean density c_0. $\mathbf{J} = e\mathbf{J}^+ - e\mathbf{J}^-$ is the electric current density. $\phi_e(t)$ is an externally imposed potential that we shall use to calculate charge–charge correlation functions. Substituting Eq. (23) for $\mathbf{J}$ in (15), we find

$$\begin{aligned}
\frac{\partial \mathbf{E}}{\partial t} = {}& \epsilon_0/\xi\nabla^2\mathbf{E} - e^2\mu c_0/\epsilon_0\mathbf{E} + (D/\epsilon_0 - 1/\xi)\,\text{grad}\,\rho\\
&+ e^2 c_0\mu/\epsilon_0\;\text{grad}\,\phi_e\,.
\end{aligned} \tag{24}$$

We analyze this equation by treating separately the longitudinal and transverse fluctuations. Take the curl of Eq. (24) to find that the transverse components of $\mathbf{E}$ decouple from the charge density. In Fourier space we find the dispersion law

$$(i\omega + \epsilon_0/\xi q^2 + e^2\mu c_0/\epsilon_0)\mathbf{q}\times\mathbf{E} = 0. \tag{25}$$

In the absence of charges the mode is diffusive but the presence of a finite charge density gives a gap in the spectrum.

Consider now the equations for the field, Eq. (24): With the help of Gauss' law one replaces the divergence of the field by the charge to find

$$\left(\frac{\partial}{\partial t} - D\nabla^2 + e^2\mu c_0/\epsilon_0\right)\rho = c_0 e^2\mu\nabla^2\phi_e\,, \tag{26}$$

which also applies to the longitudinal mode of the electric field,

$$(i\omega + Dq^2 + e^2\mu c_0/\epsilon_0)\mathbf{q}\cdot\mathbf{E} = -e^2 c_0\mu q^2\phi_e/\epsilon_0\,. \tag{27}$$

Again the spectrum has a gap as $q\to 0$.

III. NUMERICAL RESULTS

A. Dynamics

We performed simulations of a charged lattice gas to study the dynamics of the density and charge fluctuations.

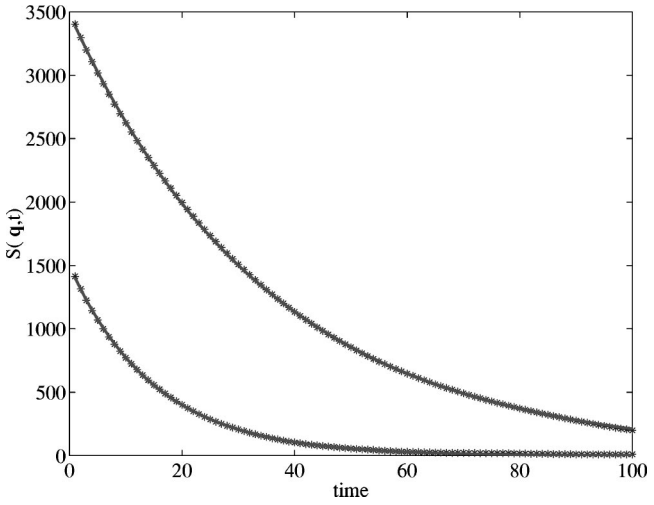

FIG. 3. Fit of a density–density, top, and a charge–charge, bottom, correlation functions, Eq. (29), to a single exponential. 5000 particles, a network of $25\times25\times25$, mode $\mathbf{q}=2\pi\times(2,2,0)$. Arbitrary units.

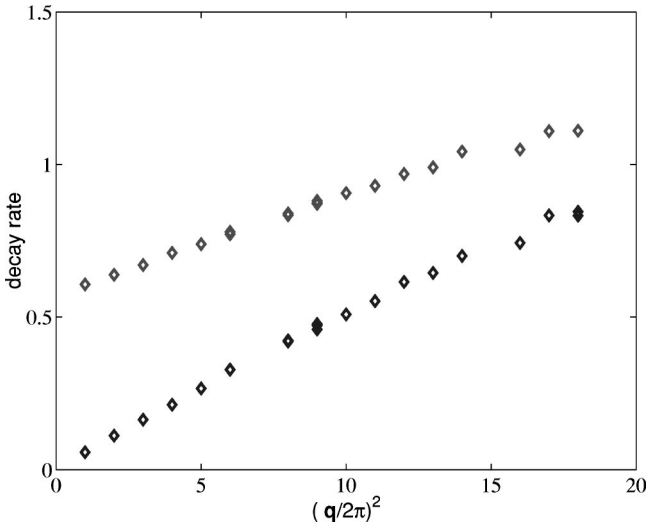

FIG. 4. Characteristic time extracted from $S(q,t)$ as a function of q^2. Bottom curve: Density–density correlations: the mode is diffusive, Eq. (23). Top curve: The charge–charge correlation function has a gap, in agreement with Eq. (26). Selected modes between $(q/2\pi)^2=1$, $\mathbf{q}=2\pi\times(1,0,0)$ and $(q/2\pi)^2=18$, $\mathbf{q}=2\pi\times(4,1,1)$. 1000 particles, $18\times18\times18$ mesh. The vertical axis is in arbitrary units.

Equal numbers of positively and negatively charged particles with $e=\pm1$ were placed on the vertices of a network which was simulated by the algorithm in a uniform dielectric background. During the simulations we measured the Fourier transform of the particle distributions,

$$s(\mathbf{q},t)=\frac{1}{\sqrt{N}}\sum_i e_i \exp(i\mathbf{r}_i(t)\cdot\mathbf{q}_i), \tag{28}$$

where the weight e_i is the charge for the charge correlation function and is unity for the density correlation function. We use this information to construct the dynamic structure factor

$$S(\mathbf{q},t)=\langle s(\mathbf{q},t)s(-\mathbf{q},0)\rangle. \tag{29}$$

The result is fitted with an exponential and the decay rate plotted as a function of q^2 in Figs. 3 and 4. The density–density correlation function displays simple diffusive behavior. The charge–charge correlation function is characterized by a gap at $q=0$.

What do these dispersion relations imply for the equilibration of a system of charged particles? The mass degree of freedom is diffusive so that a simulation equilibrates in a time which scales quadratically with the linear dimensions of the system. The charge degree of freedom is associated with a Green function which is also diffusive. However, the total weight decays exponentially in time. The signal due to a charge fluctuation is very weak beyond the Debye length.

Note that the parameters used in the derivation of the plasma dynamics are already at a coarse grained level of description. We expect that the bare parameters are renormalized by nonlinear interactions: While Eq. (15) is in some sense fundamental, containing within it the exact statement of Coulomb's law and Boltzmann statistics, Eqs. (23) are purely phenomenological. An example is the mobility of a particle μ which in the above theoretical presentation appears independent of the field parameters ϵ_0 and ξ. However, consider the case of a charged particle pulled by an external nonelectric force in the presence of an electric field which relaxes very slowly. As the particle moves it leaves behind it a "string" of electric field due to the dynamics of Fig. 1. This creates a back force on the particle which reduces its mobility. Monte-Carlo moves on the field spread this string over many lattice sites increasing the mobility of a charged particle. Thus the mobility of the charged particles increases when the field relaxes more rapidly.

This effect is an explanation of the curves of Fig. 4. Despite the predictions of Eqs. (23) and (26) the slope of the charge–charge and the density–density curves are slightly different; the effective diffusion coefficient of the charge fluctuations is lower than that of the density fluctuations. Slow relaxation of the electric degrees of freedom should hinder the motion of a single charged particle more than a strongly coupled, neutral pair moving in the same direction.

B. Screening

From the Poisson–Boltzmann equation it is known that charged systems screen. We derive this result from our dynamic equations as follows: Consider Eq. (26) for the charge density in the presence of a static external potential $\phi_e(\mathbf{q})$:

$$\rho(\mathbf{q})=\frac{-q^2}{q^2+e^2c_0/\epsilon_0k_BT}\frac{c_0e^2\phi_e}{k_BT}, \tag{30}$$

from linear response theory the structure factor with the normalization of Eq. (29) is given by

$$S(q)=\frac{e^2q^2}{\kappa^2+q^2}, \tag{31}$$

where the inverse Debye length, κ, is given by the standard expression $\kappa^2=e^2c_0/\epsilon_0k_BT$. This prediction is checked in our code by plotting $1/S(q)$ as a function of $1/q^2$, Fig. 5.

Figure 5 should be taken as very strong evidence that our algorithm is behaving correctly. It reproduces one of the

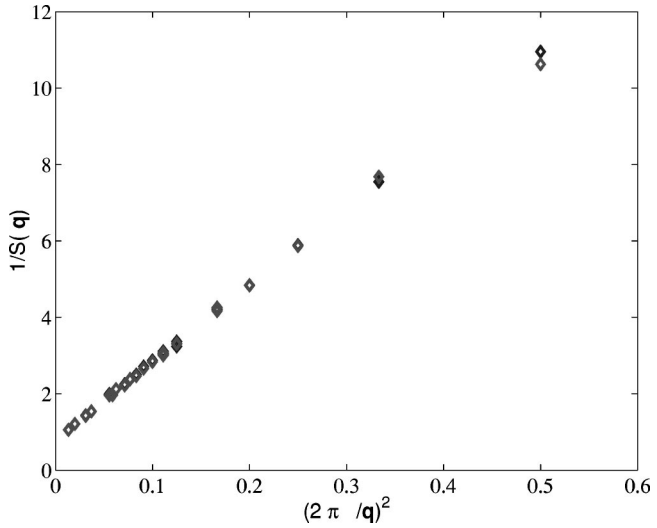

FIG. 5. A plot of $1/S(q)$ as a function of $(2\pi/q)^2$. The plot is linear as implied by Eq. (31). Selected modes between $2\pi\times(1,1,0)$ out to $2\pi\times(5,5,5)$. The plasma screens interactions exponentially. 5000 charges on a network of $25\times25\times25$.

most striking features of charged systems, the exponential decay of the charge–charge correlation function due to Debye screening.

C. Numerical stability

In the simulations that we performed to study the dynamic and screening properties of the algorithm we were agreeably surprised by the numerical stability of the algorithm: At each update one makes an error e_p comparable to the round off error of the computer. Over many time steps this accumulates so that Gauss' law is violated. We feared that this local error would rapidly become important.

The slow propagation (in time) of numerical errors can be understood by consideration of Eq. (17). Local fluctuations in the constraint $\mathrm{div}\,\mathbf{E}-\rho/\epsilon_0=0$ spread out via a diffusion process. Since both positive and negative errors are made during a simulation there is a large degree of cancellation occurring. After a single Monte-Carlo sweep of the system Gauss' law is violated by $O(e_p)$ at each lattice site. However, averaged over a sample with L^3 sites the average error per site is $O(e_p/L^{3/2})$. When simulated for $O(L^2)$ sweeps the system comes to equilibrium under the diffusive propagation of the charge and density fluctuations, we find errors of only $O(e_p/L^{1/2})$ per site. The high statistics curves of this paper were generated by using runs of length up to 5000 times the equilibration time. Even here the errors remained acceptably small.

IV. PROPAGATIVE FIELD EQUATIONS

A. Maxwell's equations

In Eq. (15) we gave the equations of motion for the electric field obeyed in the continuum limit of a Monte-Carlo simulation. In this section we shall see how local imposition of Gauss' law can be used to find a propagative dynamics for the evolution of the electric field. We continue to describe the basic dynamic degree of freedom as an angular variable, $\boldsymbol{\Theta}$, which is linked to the electric field by Eq. (13). This variable is associated with a angular velocity, $\mathbf{v}_\theta$, and moment of inertia, I_θ. The resulting second order equations will display propagating, wave like features rather than the diffusive propagation characteristic of Eq. (15).

Each link field $E_{i,j}$ is the result of the rotation of a variable $\boldsymbol{\Theta}$ defined on the faces of the cube rotating at angular velocity $\mathbf{v}_\theta$. As above the torque on the rotational degree of freedom of a plaquette is given by $\mathbf{C}=-\epsilon_0\mathrm{curl}\,\mathbf{E}$. Using Eqs. (6) and (12) we find the following equations obeyed by the fields:

$$I_\theta\frac{\partial\mathbf{v}_\theta}{\partial t}=-\epsilon_0\,\mathrm{curl}\;\mathbf{E},$$

$$\frac{\partial\mathbf{E}}{\partial t}=\mathrm{curl}\;\mathbf{v}_\theta-\mathbf{J}/\epsilon_0, \tag{32}$$

$$\mathrm{div}\,\mathbf{E}=\rho/\epsilon_0,$$

where the differential operators are to be interpreted as the appropriate difference when acting on the lattice variables. The equations (32) are a rescaled version of Maxwell's equations with $\mathbf{v}_\theta$ playing the role of the magnetic field $\mathbf{H}$.

In order to find the coupling between particles and the variables $\boldsymbol{\Theta}$ we are obliged to use the formalism of Lagrangian dynamics. Naive arguments based on energy considerations are ambiguous and can easily lead to wrong results.

B. Lagrangian treatment of dynamics

We shall now show how to derive the full coupled equations between particle motion and field. First, however, we shall look at a simple illustrative example in order bring out the main formal features of constrained Lagrangian dynamics.

Consider two gears described by the rotation angles φ and ψ. We take these gears to have unit inertia and impose on them a potential energy $g(\varphi)$ and $h(\psi)$. The gears are in contact and are thus submitted to the rolling constraint

$$\dot{\varphi}+\dot{\psi}=0. \tag{33}$$

We find that the Lagrangian describing this system is simply

$$\mathcal{L}=\frac{\dot{\varphi}^2}{2}+\frac{\dot{\psi}^2}{2}-g-h+A(\dot{\varphi}+\dot{\psi}), \tag{34}$$

where the Lagrange multiplier A imposes the constraint. Note that we are *not* using the standard method of D'Alembert of imposing nonholonomic constraints but rather the "vakonomic" method[10] in which the field A is itself considered an independent dynamic variable. Such methods are widely used in field theory; see, for instance, the book of Schwinger.[11]

From this Lagrangian we find the equations of motion and the momenta. For instance,

$$p_\varphi=\dot{\varphi}+A \tag{35}$$

and

$$\frac{d^2\varphi}{dt^2} = -\frac{dg}{d\varphi} - \frac{dA}{dt}. \tag{36}$$

These equations linking the momentum p_φ to the velocity and the equation for the acceleration of the variable φ are remarkably similar to those found in electromagnetism if one interprets A as the vector potential.

We shall now use the same trick of considering the constrained Lagrangian dynamics of the field $\mathbf{\Theta}$ to find the coupled equations for the field and moving particles. We interpret the variable $\dot{\mathbf{\Theta}}$ as a rotation velocity and $\mathbf{E}^2$ as a potential energy. For notational simplicity we consider unit mass particles and a system of units where $\epsilon_0 = I_{\mathbf{\Theta}} = 1$. We find the following Lagrangian:

$$\mathcal{L} = \sum_i \frac{\dot{\mathbf{r}}_i^2}{2} + \int d^3\mathbf{r}\left(\frac{\dot{\mathbf{\Theta}}^2}{2} - \frac{\mathbf{E}^2}{2}\right) + \int d^3\mathbf{r}\mathbf{A}\cdot\left(\dot{\mathbf{E}} - \text{curl}\ \dot{\mathbf{\Theta}} + \sum_i q_i\delta(\mathbf{r}-\mathbf{r}_i)\dot{\mathbf{r}}_i\right). \tag{37}$$

Here the Lagrange multiplier $\mathbf{A}$ imposes the kinematic constraint, Eq. (13), in a manner analogous to the rolling constraint for the gears. We find the equations of motion by the usual variational calculus: it is useful to note that the curl operator is self adjoint with appropriate boundary conditions so that $\int \mathbf{A}\cdot\text{curl}\ \mathbf{B}\ d^3\mathbf{r} = \int \mathbf{B}\cdot\text{curl}\ \mathbf{A}\ d^3\mathbf{r}$,

$$\begin{aligned}
&\delta\mathbf{\Theta}: \quad \ddot{\mathbf{\Theta}} - \text{curl}\ \dot{\mathbf{A}} = 0,\\
&\delta\mathbf{E}: \quad \mathbf{E} + \dot{\mathbf{A}} = 0,\\
&\delta\mathbf{r}_i: \quad \ddot{\mathbf{r}}_i + q_i\frac{d\mathbf{A}}{dt} - q_i\,\text{grad}\,(\dot{\mathbf{r}}_i.\mathbf{A}) = 0,\\
&\delta\mathbf{A}: \quad \dot{\mathbf{E}} - \text{curl}\ \dot{\mathbf{\Theta}} + \sum_i q_i\delta(\mathbf{r}-\mathbf{r}_i)\dot{\mathbf{r}}_i = 0.
\end{aligned} \tag{38}$$

The variation in $\delta\mathbf{r}_i$ can be rewritten by using the identity $\text{grad}(\mathbf{v}.\mathbf{A}) = (\mathbf{v}.\text{grad})\mathbf{A} + \mathbf{v}\times\text{curl}\ \mathbf{A}$ and by noting that $d/dt = (\partial/\partial t + \mathbf{v}.\text{grad})$,

$$\begin{aligned}
&\ddot{\mathbf{r}}_i + q_i\dot{\mathbf{A}} - q_i\dot{\mathbf{r}}_i\times\text{curl}\ \mathbf{A} = 0,\\
&\ddot{\mathbf{r}}_i = q_i(\mathbf{E} + \dot{\mathbf{r}}_i\times\text{curl}\ \dot{\mathbf{\Theta}}).
\end{aligned} \tag{39}$$

These are the normal equations of electromagnetism if we identify $\dot{\mathbf{\Theta}}$ with $\mathbf{B}$. The Lagrangian corresponds to the *temporal gauge* where the scalar potential $\phi = 0$. A gauge transformation $\mathbf{A} \to \mathbf{A} + \text{grad}\,\Psi(t)$ generates additional terms in the Lagrangian of the form $\phi(\text{div}\,\mathbf{E} - \rho)$ with $\phi = \partial\Psi/\partial t$.

We can eliminate $\dot{\mathbf{\Theta}}$ from the Lagrangian via the Thomson–Routh treatment of kinesthenic variables: Consider the modified action $\overline{\mathcal{L}} = \mathcal{L} - \mathbf{p}_\theta\cdot\dot{\mathbf{\Theta}}$. We find that

$$\overline{\mathcal{L}} = \sum_i \frac{\dot{\mathbf{r}}_i^2}{2} - \int d^3\mathbf{r}\left(\frac{(\text{curl}\ \mathbf{A})^2}{2} + \frac{\mathbf{E}^2}{2}\right) + \int d^3\mathbf{r}\mathbf{A}\cdot(\dot{\mathbf{E}} + \mathbf{J}), \tag{40}$$

which we recognize[11] as a more conventional Lagrangian for electrodynamic systems.

We construct the Hamiltonian using Dirac's procedure with two constraints:

$$\mathcal{H} = \sum_i \frac{(\mathbf{p}_i - q_i\mathbf{A}(\mathbf{r}_i))^2}{2} + \int \frac{(\mathbf{p}_\theta + \text{curl}\ \mathbf{A})^2}{2} d^3\mathbf{r} + \int\left(\frac{\mathbf{E}^2}{2} + \mu\mathbf{p}_\mathbf{A} + \gamma(\mathbf{p}_\mathbf{E} - \mathbf{A})\right) d^3\mathbf{r}, \tag{41}$$

where $\mu = \mathbf{E}$, $\gamma = \dot{\mathbf{E}}$. The initial conditions are $\mathbf{p}_E = \mathbf{A}$, $\mathbf{p}_A = 0$ and $\mathbf{p}_\theta = 0$ which are conserved by the equations of motion in the same way that Gauss' law is conserved in the Monte-Carlo formulation. On the physically relevant surface the constraint terms are identically zero; the extended Hamiltonian still has the normal interpretation as the conserved total energy.

Such a description of the electromagnetic field in terms of rotors was known to FitzGerald in the nineteenth century as a mechanical analogy[12,13] of the ether. A square array of wheels was constructed; neighboring wheels were connected by an elastic band. When two neighboring wheels turn at the same angular velocity the elastic band has constant length and the elastic energy is constant. When there is a difference of rotational velocity between wheels the elastic energy of the bands changes. Assuming linear elasticity for the elastic bands one finds an exact mapping of electromagnetism onto a mechanical problem. This model was most important in the history of electromagnetism: FitzGerald used this model in the very first calculation of radiated power from moving charges.

C. Statistical mechanics

The interpretation of $\dot{\mathbf{\Theta}}$ as the angular velocity of a rotor suggests that it could be coupled to a thermostat to improve equilibration of the field degrees of freedom; the linear equations that we have found for the electric field are likely to equilibrate rather slowly. If we add coupling to external noise, $\vec{\zeta}$ and friction, Γ, in Eq. (38), we find

$$\ddot{\mathbf{\Theta}} = \text{curl}\ \dot{\mathbf{A}} - \Gamma\dot{\mathbf{\Theta}} + \vec{\zeta}(t), \tag{42}$$

thus coupling the angular velocity to an arbitrary thermostat leads to violation of the Maxwell equation $\text{div}\,\mathbf{B} = 0$.

The partition function is calculated from

$$\mathcal{Z} = \int \mathcal{D}\mathbf{p}\mathcal{D}\mathbf{q}e^{-\beta\mathcal{H}}. \tag{43}$$

The integral is over the canonical coordinates $\mathbf{q}$ and momenta $\mathbf{p}$. The integration region is the set of configurations available to the equations of motion. We thus implicity include delta function constraints on $\mathbf{p}_E$ and $\mathbf{p}_A$. Integration over the momenta is easy to perform in the presence of Langevin noise which destroys the constraints and conservation laws associated with the variable $\mathbf{p}_\theta$ in Maxwell's equations. What remains is the integral over the electric fields and particle positions. If the dynamics were ergodic we would integrate over all values of the field. However, Maxwell's equations, even in the presence of noise on the momentum degree of freedom, include Gauss' law. This constrains the electric field and the partition function is given by

$$\mathcal{Z}_c = \int \mathcal{D}\mathbf{r}_i \int \mathcal{D}\mathbf{E} e^{-\int (\beta\epsilon_0 \mathbf{E}^2/2) \mathrm{d}^3\mathbf{r}} \prod_{\mathbf{r}} \delta(\mathrm{div}\,\mathbf{E} - \rho/\epsilon_0), \tag{44}$$

where, now, all degrees of freedom are freely integrated over. It is this constrained configurational integral[7] that leads to effective Coulomb interactions.

Combining Eqs. (13) and (42) we find the equation for the electric field:

$$\frac{\partial}{\partial t}\left(\frac{\partial}{\partial t} + \Gamma\right)\mathbf{E} = \nabla^2\mathbf{E} - \mathrm{grad}\,\rho - \left(\Gamma + \frac{\partial}{\partial t}\right)\mathbf{J} + \mathrm{curl}\ \vec{\zeta}(t). \tag{45}$$

In the limit of low frequencies we can ignore $\partial/\partial t$ compared to Γ and find an equation entirely equivalent to Eq. (15). The damping strongly modifies the large scale nature of the electric field dynamics.

This result seems quite remarkable. It is known from the work of Heaviside[14] that the electric field of a moving particle is strongly modified at velocities which approach c, the speed of light. Despite this, Eq. (44) implies that the average interaction between particles is independent of this longitudinal contraction of the electric field. Either this is a consequence of the full Maxwell equations which has not yet been or explored or it is a consequence of relaxing the constraint on the divergence of the magnetic field leading to the modified large scale properties implied in Eq. (45). We leave the further study of this problem to a future publication. In either case this could permit the study of the Coulomb interacting particles via direct integration of the Maxwell equations in molecular dynamics simulations.

V. CONCLUSIONS

We have analyzed a Monte-Carlo algorithm for the simulation of long ranged Coulomb interactions. We have seen that propagation of the electric degrees of freedom is diffusive. By construction the dynamics sample the equilibrium Boltzmann distribution of the charged system. The locality of the algorithm allows fast and *simple* implementations even on multiprocessor computers with high communication overheads. We have verified that the Monte-Carlo algorithm reproduces well known features of the two component plasma such as screening. Our law for the *local* update of the electric field after movement of a particle, Fig. 1, is a discretized version of the Maxwell displacement current. The algorithm has been shown to be closely related to mechanical models of the ether introduced in the generation that followed Maxwell.

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