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Variational formulation of macro-particle plasma simulation algorithms[a]

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A variation formulation of macro-particle kinetic plasma models is discussed. In the electrostatic case, the use of symplectic integrators is investigated and found to offer advantages over typical generic methods. For the electromagnetic case, gauge invariance and momentum conservation are considered in detail. It is shown that, while the symmetries responsible for these conservation laws are broken in the presence of a spatial grid, the conservation laws hold in an average sense. The requirements for exact invariance are explored and it is shown that one viable option is to represent the potentials with a truncated Fourier basis. © 2014 AIP Publishing LLC.
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I. INTRODUCTION

Often a complete microscopic physical description of a large dynamical system simply contains too much information. This unwanted information can arise from a variety of sources. For example, many of the degrees-of-freedom may be devoted to describing small departures from a common behavior; the system may contain time-scales that are not of interest; or a complete description results in an unrealistic computational burden. Variational methods are well suited to removing information while retaining key structural aspects of the system (such as conservation laws). Plasma systems, with their diverse range of phenomena, can possess any combination of these characteristics. Here, we are concerned primarily with the case of the full description being computationally infeasible. In particular, we focus on the Vlasov–Maxwell system, which, on the full six-dimensional phase space, is computationally intractable.

Macro-particle methods are widely used for modeling kinetic plasmas with a manageable (in most cases) computational cost. In the main, these algorithms are formulated by approximating the continuous equations of motion. For systems governed by a variational principle (such as collisionless plasmas), approximations of the equations of motion are known to introduce anomalous behavior especially in system invariants. Recently, a variational formulation of macro-particle plasma models, based on a reduction of the distribution function, has been developed.[1] As in the usual Particle-In-Cell (PIC) formulation,[2–4] these macro-particles have a definite momentum and are spatially extended. The primary advantage of this approach is the preservation of the link between symmetries and conservation laws. Further, the variational formulation allows for constructing models of arbitrary spatial and temporal order. In contrast, the overall accuracy of the usual PIC algorithm is at most second due to the nature of the force interpolation between the gridded field quantities and the (continuous) particle position. The

variational algorithm has essentially the same computational cost per particle update as the usual PIC method. However, the variational method uses the potentials directly to evaluate forces (as opposed to using the fields) and, empirically,[5] appears to have much reduced levels of numerical noise. Moreover, since the equations of motion are derived from a finite degree-of-freedom Lagrangian, it is possible to construct a canonical Hamiltonian system, allowing the use of symplectic integration algorithms. In Sec. III, we demonstrate the advantages of symplectic integrators for a simple test case of weak Landau damping.

The extension of the techniques of Ref. 1 to the electromagnetic case is relatively straightforward.[5] In Sec. IV, we examine in detail the requirements for gauge invariance and momentum conservation in the discrete system and show the connection to the discrete continuity equation. For reductions representing the potentials on a spatial grid, we show that, in general, the discrete version of the continuity equation is only satisfied in an average sense. The continuity equation is embodied in the reduction of the distribution function and not obtained from the variational principle; as a result, it typically suffers truncation errors when a discrete spatial representation is introduced. We develop requirements for an exact discrete representation of the continuity equation and show that a truncated Fourier expansion of the potentials satisfies these requirements, leading to exact gauge invariance and momentum conservation.

II. A PHASE SPACE REDUCTION

We begin with a review of the reduction procedure developed by Evstatiev and Shadwick.[1] For simplicity, we consider a single mobile plasma species and restrict our discussion to the electrostatic case. We will consider an electromagnetic extension in Sec. IV below. The central idea is to replace the phase-space distribution function f with N_p spatially extended macro-particles, each having a definite momentum

$$f(x, v, t) = \sum_{\alpha=1}^{N_p} w_\alpha S[x - \xi_\alpha(t)] \, \delta[v - \dot{\xi}_\alpha(t)], \quad (1)$$

where ξ_α is the macro-particle location, S is the macro-particle spatial distribution, normalized by $\int dx\, S(x - \xi_\alpha) = 1$, w_α is the macro-particle weight (the number of real particles represented by the corresponding macro-particle) with the total number of particles given by $\sum_{\alpha=1}^{N_p} w_\alpha$, and $\delta(v)$ is the Dirac δ-function. For a plasma species with charge q_s, we define the charge and current densities $\mathcal{N}$ and $\mathcal{J}$, respectively, as

$$\mathcal{N} = q_s \int dv\, f = q_s \sum_{\alpha=1}^{N_p} w_\alpha\, S[x - \xi_\alpha(t)] \qquad (2a)$$

and

$$\mathcal{J} = q_s \int dv\, vf = q_s \sum_{\alpha=1}^{N_p} w_\alpha\, \dot\xi_\alpha\, S[x - \xi_\alpha(t)]. \qquad (2b)$$

Now

$$\frac{\partial \mathcal{N}}{\partial t} = q_s \sum_{\alpha=1}^{N_p} w_\alpha\, \dot\xi_\alpha\, \frac{\partial}{\partial \xi_\alpha} S[x - \xi_\alpha(t)]$$

$$= -q_s \sum_{\alpha=1}^{N_p} w_\alpha\, \dot\xi_\alpha\, \frac{\partial}{\partial x} S[x - \xi_\alpha(t)] = -\frac{\partial \mathcal{J}}{\partial x}; \qquad (3)$$

hence this representation exactly preserves the continuity equation. The continuity equation is a consequence of $\partial S/\partial x = -\partial S/\partial \xi_\alpha$, which trivially follows from the macro-particle spatial density $S[x - \xi_\alpha(t)]$. It is straightforward to show that existence of an exact continuity equation guarantees both gauge invariance and, in an unbounded system, exact momentum conservation. We will return to this point in Sec. IV.

Substituting (1) into Low's Lagrangian[6] yields

$$\mathcal{L} = \frac{m_s}{2} \sum_{\alpha=1}^{N_p} w_\alpha\, \dot\xi_\alpha^2 - q_s \sum_{\alpha=1}^{N_p} w_\alpha \int dx\, S(x - \xi_\alpha)\, \varphi(x)$$

$$+ \frac{1}{8\pi} \int dx (\nabla \varphi)^2, \qquad (4)$$

where m_s is the species mass and $\varphi(x)$ is the electrostatic potential (the reader is directed to Ref. 1 for the details of this calculation). It is desirable to introduce a grid to aid in computing the potential but this necessarily requires constructing the potential between the grid points to evaluate the coupling term $\int dx\, S(x - \xi_\alpha)\, \varphi(x)$. This can be done to any desired accuracy using finite-elements. We take a uniform spatial grid x_i with $i \in [1, N_g]$ and grid spacing Δx and denote the numerical approximation of $\varphi(x_i)$ by φ_i. Let $\Psi_i(x)$, $i = 1,\ldots,N_g$ be a finite-element basis of some order. With this basis, we approximate φ as

$$\hat\varphi(x) = \sum_{i=1}^{N_g} \varphi_i \Psi_i(x). \qquad (5)$$

By construction, the basis vectors are only non-zero at a single grid-point, $\Psi_i(x_j) = \delta_{ij}$, and thus this representation of φ

preserves the values at the grid-points, i.e., $\hat\varphi(x_k) = \varphi_k$. With this approximation, the coupling term in $\mathcal{L}$ becomes

$$\int dx\, S(x - \xi_\alpha)\, \hat\varphi(x) = \sum_{i=1}^{N_g} \varphi_i \int dx\, S(x - \xi_\alpha) \Psi_i(x)$$

$$= \sum_{i=1}^{N_g} \varphi_i\, \rho_i(\xi_\alpha), \qquad (6)$$

where

$$\rho_i(\xi_\alpha) = \int dx\, S(x - \xi_\alpha) \Psi_i(x) \qquad (7)$$

is the projected shape of the macro-particle. For a given choice of basis and particle shape S, the expression for ρ_i can be computed analytically.

It remains to approximate the field energy term in (4). Here, we may either use the same finite element representation used to compute the coupling[7] or we can employ finite differences. In either case, we can write[1]

$$\int dx (\nabla \varphi)^2 \approx -\Delta x \sum_{i,j=1}^{N_g} \varphi_i\, \mathcal{K}_{ij}\, \varphi_j. \qquad (8)$$

When this term is approximated using finite elements, $\mathcal{K}_{ij}$ is naturally symmetric. When using finite differences, it is reasonable to first integrate by parts; one must then introduce a finite difference representation for the second derivative. There is no particular reason to use central differencing to approximate this derivative; however, from the structure of (8), we see that only the symmetric part of $\mathcal{K}$ contributes to the Lagrangian. Thus regardless of the nature of the finite difference approximation, the effective differencing operator in the Lagrangian always corresponds to some central difference approximation. Thus the discrete equations retain the self-adjoint property of the continuous system. This observation holds even if one chooses not to integrate-by-parts.[5] To avoid ambiguity, henceforth we assume that $\mathcal{K}$ corresponds to a central difference.

We now arrive at the finite degree-of-freedom Lagrangian

$$\mathcal{L} = \frac{m_s}{2} \sum_{\alpha=1}^{N_p} w_\alpha\, \dot\xi_\alpha^2 - q_s \sum_{\alpha=1}^{N_p} \sum_{i=1}^{N_g} w_\alpha \rho_i(\xi_\alpha)\, \varphi_i$$

$$- \frac{\Delta x}{8\pi} \sum_{i,j=1}^{N_g} \varphi_i\, \mathcal{K}_{ij}\, \varphi_j. \qquad (9)$$

The equations of motion are obtained in the usual way by demanding the action be stationary, viz.

$$\ddot\xi_\alpha = -\frac{q_s}{m_s} \sum_{i=1}^{N_g} \frac{\partial \rho_i(\xi_\alpha)}{\partial \xi_\alpha} \varphi_i \qquad (10a)$$

and

$$\sum_{j=1}^{N_g} \mathcal{K}_{ij} \varphi_j = -\frac{4\pi q_s}{\Delta x} \sum_{\alpha=1}^{N_p} w_\alpha\, \rho_i(\xi_\alpha). \qquad (10b)$$

From Poisson's equation, we see that $w_\alpha \rho_i(\xi_\alpha)$ represents the density on the grid due to each macro-particle. If the $\Psi_i(x)$ used in the interpolation are constructed from Lagrange polynomials, then $\sum_{i=1}^{N_g} \Psi_i(x) = 1$ and

$$\sum_{i=1}^{N_g} \rho_i(\xi_\alpha) = \sum_{i=1}^{N_g} \int dx\, S(x - \xi_\alpha) \Psi_i(x)$$
$$= \int dx\, S(x - \xi_\alpha) = 1. \tag{11}$$

That is, at any instant, the total system charge (represent by the N_p macro-particles) is fully deposited onto the grid. Since our discrete Lagrangian is time independent, this system has a conserved energy that takes the form[1]

$$W_L = \frac{m_s}{2} \sum_{\alpha=1}^{N_p} w_\alpha \dot{\xi}_\alpha^2 - \frac{\Delta x}{8\pi} \sum_{i,j=1}^{N_g} \varphi_i \mathcal{K}_{ij} \varphi_j. \tag{12}$$

In the electrostatic approximation, φ is not dynamical, i.e., $\dot{\varphi}_i$ does not appear in the Lagrangian; and hence, φ_i is completely determined by the instantaneous charge density. Thus, we may view φ_i as a known function of ξ_α, defined by (10b). As a result, we can perform the Legendre transform to obtain a canonical Hamiltonian system. The macro-particle momentum is defined as $\pi_\alpha = \partial \mathcal{L} / \partial \dot{\xi}_\alpha = m_s w_\alpha \dot{\xi}_\alpha$ leading to the Hamiltonian

$$\mathcal{H} = \sum_{\alpha=1}^{N_p} \pi_\alpha \dot{\xi}_\alpha - \mathcal{L}$$
$$= \frac{1}{2m_s} \sum_{\alpha=1}^{N_p} \frac{\pi_\alpha^2}{w_\alpha} + q_s \sum_{\alpha=1}^{N_p} \sum_{i=1}^{N_g} w_\alpha \rho_i(\xi_\alpha) \varphi_i + \frac{\Delta x}{8\pi} \sum_{i,j=1}^{N_g} \varphi_i \mathcal{K}_{ij} \varphi_j$$
$$= \frac{1}{2m_s} \sum_{\alpha=1}^{N_p} \frac{\pi_\alpha^2}{w_\alpha} - \frac{\Delta x}{8\pi} \sum_{i,j=1}^{N_g} \varphi_i \mathcal{K}_{ij} \varphi_j, \tag{13}$$

where in the last step we have used (10b). This Hamiltonian is equivalent to the energy expression in (12) (of course, $\mathcal{H}$ is a function of ξ_α and π_α while W_L depends on ξ_α and $\dot{\xi}_\alpha$). From the Hamiltonian, we find

$$\dot{\xi}_\alpha = \frac{\pi_\alpha}{m_s w_\alpha}, \tag{14a}$$

$$\dot{\pi}_\alpha = \frac{\Delta x}{4\pi} \sum_{i,j=1}^{N_g} \varphi_i \mathcal{K}_{ij} \frac{\partial \varphi_j}{\partial \xi_\alpha}$$
$$= \frac{\Delta x}{4\pi} \sum_{i=1}^{N_g} \varphi_i \left(-\frac{4\pi q_s}{\Delta x} \right) \frac{w_\alpha \partial \rho_i(\xi_\alpha)}{\partial \xi_\alpha}$$
$$= -q_s w_\alpha \sum_{i=1}^{N_g} \varphi_i \frac{\partial \rho_i(\xi_\alpha)}{\partial \xi_\alpha}. \tag{14b}$$

One can readily see that (14a) and (14b) are equivalent to (10a).

Evstatiev and Shadwick[1] also derive a noncanonical Hamiltonian formulation in terms of the electric field, resulting in the equations of motion

$$\dot{\xi}_\alpha = \frac{\pi_\alpha}{m_s w_\alpha}, \tag{15a}$$

$$\dot{\pi}_\alpha = q_s w_\alpha \sum_{i=1}^{N_g} E_i \rho_i(\xi_\alpha), \tag{15b}$$

$$\dot{E}_i = -\frac{4\pi q_s}{\Delta x} \sum_{\alpha=1}^{N_p} \frac{\pi_\alpha}{m_s} \rho_i(\xi_\alpha), \tag{15c}$$

where E_k is the numerical approximation to the electric field at x_k. In this case, the conserved energy (the non-canonical Hamiltonian) is

$$W_H = \frac{1}{2m_s} \sum_{\alpha=1}^{N_p} \frac{\pi_\alpha^2}{w_\alpha} + \frac{1}{8\pi} \sum_{i=1}^{N_g} E_i^2. \tag{16}$$

III. TIME INTEGRATION

The above formulation treats time as a continuous variable. Of course, performing numerical computations with these models naturally requires discretization in time. By keeping time continuous in the variational principle (as opposed, say, to fully discretizing the action[8]), the flexibility to tailor the time-integration to the problem at hand is retained. This is particularly important in the electromagnetic case,[5] where stability considerations[9] typically dictate the temporal integration order depending on the spatial approximation. Here, we consider various integration schemes, providing numerical examples for two explicit methods and exploring properties of an implicit method. We assume a fixed time-step Δt and denote the numerical approximation to the macro-particle trajectory at $t_n = n \Delta t$ by ξ_α^n.

A. Time-explicit methods

The most straightforward approach to integrating (10) is to use some Runge–Kutta method; here, we will consider a second-order method. The full update involves two steps:

$$\tilde{\xi}_\alpha = \xi_\alpha^n + \frac{1}{2} \Delta t\, v_\alpha^n,$$
$$\tilde{v}_\alpha = v_\alpha^n - \frac{1}{2} \Delta t \frac{q_s}{m_s} \sum_{i=1}^{N_g} \rho_i'(\xi_\alpha^n) \varphi_i[\xi^n],$$
$$\xi_\alpha^{n+1} = \xi_\alpha^n + \Delta t\, \tilde{v}_\alpha, \tag{17}$$
$$v_\alpha^{n+1} = v_\alpha^n - \Delta t \frac{q_s}{m_s} \sum_{i=1}^{N_g} \rho_i'(\tilde{\xi}_\alpha) \varphi_i[\tilde{\xi}],$$

where $v_\alpha = \dot{\xi}_\alpha$, $\rho_i' = \partial \rho_i / \partial \xi$, and the notation $\varphi_i[\xi]$ denotes the potential, obtained from (10b), based on a particular set of macro-particle coordinates. Assuming the potential is correct at the beginning of the update, (17) requires two force-interpolations, two charge-depositions, and two field solves per step. (The last field solve necessary so that the potential is correct at the beginning of the next time-step.) This method does not exactly conserve energy, but as was shown in Ref. 1, the energy error is a function only of time-step (since the continuous-time equations are exactly

conservative). Empirically, one finds that with small enough Δt, the energy growth is approximately linear in time.

Since we can construct a canonical Hamiltonian system, it is also possible to use a symplectic integrator[10] for the time-advance. For example, applying the velocity-Verlet method[11,12] to (14), we have the following second-order time-advance:

$$\tilde{v}_\alpha = v_\alpha^n - \frac{1}{2} \Delta t \, \frac{q_s}{m_s} \sum_{i=1}^{N_g} \rho_i'(\xi_\alpha^n) \, \varphi_i[\xi^n],$$

$$\xi_\alpha^{n+1} = \xi_\alpha^n + \Delta t \, \tilde{v}_\alpha^n, \qquad (18)$$

$$v_\alpha^{n+1} = \tilde{v}_\alpha - \frac{1}{2} \Delta t \, \frac{q_s}{m_s} \sum_{i=1}^{N_g} \rho_i'(\xi_\alpha^{n+1}) \, \varphi_i[\xi^{n+1}].$$

Assuming the potential is correct at the beginning of the update, (18) requires two force-interpolations, one charge-deposition, and one field solve per step. This is more efficient than the Runge–Kutta method of the same order by saving a charge-deposition and field-solve. In addition, no intermediate storage is needed for the macro-particle phase-space, which leads to a significant reduction in memory usage. This method does not exactly conserve energy, but the energy error oscillates about the correct value (as is typical of symplectic integrators). We have verified that the amplitude of the energy oscillation scales, as expected, with Δt^2.

To illustrate the advantages of the symplectic integrator over the generic method, we consider the problem of weak (linear) Landau damping[13] where the wave-particle resonance occurs at velocities much greater than the thermal velocity. This is a particularly hard problem for a macro-particle method as only macro-particles in the tail of the distribution participate in the wave-particle resonance; the majority of the macro-particles are consigned to representing the thermal state and are not resonant. Since all macro-particles represent the same number of electrons,[14] when only a small number of macro-particles are involved in the resonance, it is challenging to correctly capture the energy transfer from fields to particles (and thus the correct damping rate). Initially, the plasma has a uniform density n_0 and is in thermal equilibrium with temperature T_0 satisfying $k_B T_0/m_s c^2 = 1/5$, where k_B is Boltzmann's constant. We take periodic boundary conditions in space, a domain size of $L = 4\pi c/\omega_p$ spanning 1024 cells, where $\omega_p = \sqrt{4\pi q_s^2 n_0/m_s}$ is the plasma frequency. These parameters were chosen to allow only a single weakly damped mode. The macro-particles are loaded in the center of the cell while the velocities are chosen randomly from a Gaussian distribution with variance $k_B T_0/m_s c^2$. At each spatial location, the macro-particle velocity distribution is shifted and scaled to have zero mean and variance exactly corresponding to T_0. The macro-particle spatial distribution S is taken to be a two-cell wide tent-function, giving cubic ρ_k (see Table A.1 of Ref. 1 for the corresponding expressions for ρ_k). Initially, we excite the $n = 2$ spatial mode of the electric field with initial amplitude E_0 given by $q_s E_0/(m_s c \, \omega_p) = 0.05$ by perturbing the macro-particle positions.

We provide an independent (and presumably more accurate) solution to this problem using an Eulerian

Vlasov–Poisson solver known to have excellent conservation properties.[15] We take identical initial conditions and spatial grid, a velocity grid spanning $-2 < v/c < 2$ with 401 grid-points with the distribution function vanishing at the limits of the velocity domain, and time-step $\omega_p\Delta t = 0.1$. With these parameters, the Vlasov–Poisson solution was sufficiently well converged that further refinements led to much smaller changes in this solution than the differences between this solution and any of the macro-particle solutions considered.

Figure 1 shows the amplitude of the $n = 2$ spatial Fourier mode of the electric field, $|\tilde{E}_2|$, in units of $m_s c^2/q_s$ obtained from three methods [Vlasov–Poisson solver, (black); symplectic integrator, (18), (red); and the Runge–Kutta integrator, (17), (blue)], where the number of macro-particles is varied. Each panel is labeled with the number of macro-particles used at each point in space, n_v, to represent the velocity distribution. While the cases with $n_v = 400$ and $n_v = 800$ show disagreement between the Runge–Kutta and symplectic integrator solution, the discrepancies are not significant as they are smaller than the overall disagreement with the Vlasov solution. For $n_v = 1600$ (bottom), the macro-particle results closely track each other and the full kinetic solution through $\omega_p t = 30$ and give good qualitative agreement over the remainder of the evolution. Not only is this more macro-particles per cell than velocity grid-points used in the Eulerian method, the computational cost of the macro-particle solution is approximately 4 times greater than that of the fully kinetic solution. (In all cases,
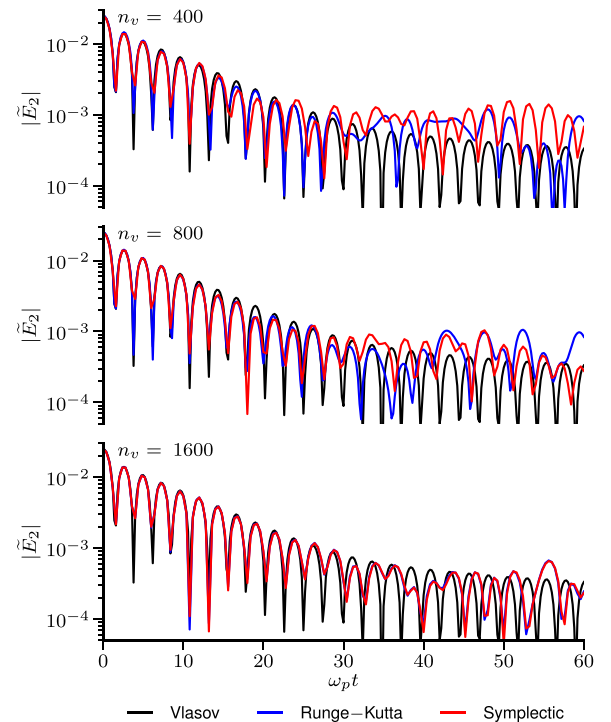

FIG. 1. Amplitude of the $n = 2$ spatial Fourier mode of the electric field in the weak Landau damping problem, computed with all three methods: Vlasov–Poisson solver, (black); symplectic integrator, (18), (red); and the Runge–Kutta integrator, (17), (blue). Each panel is labeled with the number of macro-particles, n_v, used at each point in space to represent the velocity distribution. The Vlasov–Poisson solution (black) is identical in all panels. In all cases, $\omega_p\Delta t = 0.1$ and the mode amplitude is plotted in units of $m_s c^2/q_s$.

the codes have been carefully optimized, so we believe this ratio reflects the intrinsic costs of the algorithms and is not significantly influenced by implementation details.) By further increasing n_v, it is reasonable to expect that the macro-particle solutions will exhibit better agreement with the Vlasov solution for $\omega_p t > 30$.

Figure 2 shows $|\tilde{E}_2|$ in units of $m_s c^2/q_s$ obtained from the three methods [Vlasov–Poisson solver, (black); symplectic integrator, (18), (red); and the Runge–Kutta integrator, (17), (blue)], where $n_v = 1600$ and the value of Δt used in the macro-particle integrators is varied. As the time-step is increased, the disparity between the symplectic integrator solution and the Vlasov solution increases only slightly, whereas the Runge–Kutta integrator shows marked disagreement for $\omega_p \Delta t \geq 0.4$. This significant disagreement between the macro-particle methods is rather surprising since symplectic integrators are commonly held to be only strictly necessary when following a very large number of orbits; here we consider less than 10 plasma periods. It is likely that the energy behavior of the symplectic method (i.e., oscillation versus secular growth), more than its phase-space preserving properties, is responsible for the method's superior performance. Taking into account the relative sizes of Δt needed by each method to give accurate solutions and the effort per time-step, the

symplectic method is approximately 5–10 times more computationally efficient than the generic Runge–Kutta method.

B. Time-implicit methods

Time-implicit methods for macro-particle simulations are of interest due to the prospect of exact energy conservation even with discrete time.[16,17] Applying the mid-point rule to (15), we obtain the following second-order time-advance:

$$\xi_\alpha^{n+1} - \xi_\alpha^n = \Delta t \frac{\pi_\alpha^{n+1} + \pi_\alpha^n}{2 m_s w_\alpha}, \tag{19a}$$

$$\pi_\alpha^{n+1} - \pi_\alpha^n = \frac{\Delta t}{4} q_s w_\alpha \sum_{i=1}^{N_g} \left(E_i^{n+1} + E_i^n\right) \\ \times \left[\rho_i(\xi_\alpha^{n+1}) + \rho_i(\xi_\alpha^n)\right], \tag{19b}$$

$$E_i^{n+1} - E_i^n = -\pi \frac{\Delta t}{\Delta x} \frac{q_s}{m_s} \sum_{i=1}^{N_g} \left(\pi_\alpha^{n+1} + \pi_\alpha^n\right) \\ \times \left[\rho_i(\xi_\alpha^{n+1}) + \rho_i(\xi_\alpha^n)\right], \tag{19c}$$

where E_j^n is the numerical approximation to $E(t_n, x_j)$. Considering the difference in energy at t_{n+1} and t_n, we find

$$W_H^{n+1} - W_H^n$$
$$= \frac{1}{2 m_s} \sum_{\alpha=1}^{N_p} \frac{(\pi_\alpha^{n+1} + \pi_\alpha^n)(\pi_\alpha^{n+1} - \pi_\alpha^n)}{w_\alpha}$$
$$+ \frac{\Delta x}{8\pi} \sum_{i=1}^{N_g} \left(E_i^{n+1} + E_i^n\right)\left(E_i^{n+1} - E_i^n\right)$$
$$= \frac{1}{2 m_s} \sum_{\alpha=1}^{N_p} \frac{(\pi_\alpha^{n+1} + \pi_\alpha^n)}{w_\alpha} \frac{\Delta t}{4} q_s w_\alpha \sum_{i=1}^{N_g} \left(E_i^{n+1} + E_i^n\right)$$
$$\times \left[\rho_i(\xi_\alpha^{n+1}) + \rho_i(\xi_\alpha^n)\right] - \frac{\Delta x}{8\pi} \sum_{i=1}^{N_g} \left(E_i^{n+1} + E_i^n\right)\pi \frac{\Delta t}{\Delta x}$$
$$\times \frac{q_s}{m_s} \sum_{i=1}^{N_g} \left(\pi_\alpha^{n+1} + \pi_\alpha^n\right)\left[\rho_i(\xi_\alpha^{n+1}) + \rho_i(\xi_\alpha^n)\right]$$
$$= \Delta t \frac{q_s}{8 m_s} \sum_{\alpha=1}^{N_p} \left(\pi_\alpha^{n+1} + \pi_\alpha^n\right) \sum_{i=1}^{N_g} \left(E_i^{n+1} + E_i^n\right)$$
$$\times \left[\rho_i(\xi_\alpha^{n+1}) + \rho_i(\xi_\alpha^n)\right] - \Delta t \frac{q_s}{8 m_s} \sum_{i=1}^{N_g} \left(E_i^{n+1} + E_i^n\right)$$
$$\times \sum_{i=1}^{N_g} \left(\pi_\alpha^{n+1} + \pi_\alpha^n\right)\left[\rho_i(\xi_\alpha^{n+1}) + \rho_i(\xi_\alpha^n)\right]$$
$$= 0. \tag{20}$$

That is, the mid-point rule exactly conserves the system energy; this is an example of the well-known property of the mid-point rule regarding quadratic invariants. With the mid-point rule, there is some freedom in discretizing nonlinear terms; had we written the right-hand sides of (19b) and (19c) as $E_i^{n+1}\rho_i(\xi_\alpha^{n+1}) + E_i^n \rho_i(\xi_\alpha^n)$ and $\pi_\alpha^{n+1}\rho_i(\xi_\alpha^{n+1}) + \pi_\alpha^n \rho_i(\xi_\alpha^n)$, respectively, then W_H would not have been exactly conserved. Examining the computational performance of this method will
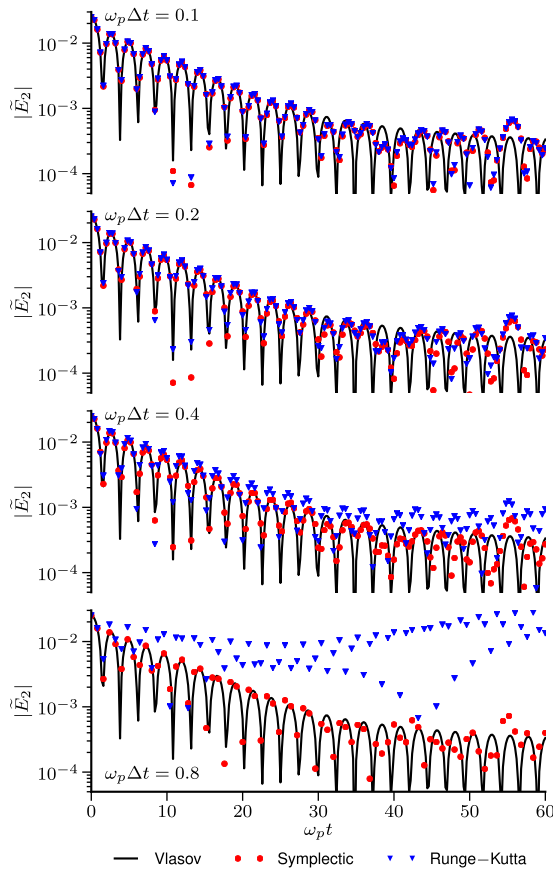

FIG. 2. Amplitude of the $n = 2$ spatial Fourier mode of the electric field in the weak Landau damping problem, computed with all three methods: Vlasov–Poisson solver, (black); symplectic integrator, (18), (red); and the Runge–Kutta integrator, (17), (blue). Each panel is labeled with the value of Δt used by the macro-particle integrators in the computation. The Vlasov–Poisson solution (black) is identical in all panels and was computed with $\omega_p \Delta t = 0.1$. In all cases, $n_v = 1600$ and the mode amplitude is plotted in units of $m_s c^2/q_s$.

be the subject of future investigations. Interestingly, in the relativistic case, with proper treatment of the nonlinear term, the mid-point method also exactly conserves energy.

It is also possible to construct an explicit integrator along the lines of Ref. 18 that exactly conserves W_H.[19] It does not appear possible to construct either implicit or explicit integration schemes that exactly conserved energy for either the Lagrangian, (10), or canonical Hamiltonian, (14), equations of motion.

IV. THE ELECTROMAGNETIC CASE: GAUGE INVARIANCE, CHARGE, AND MOMENTUM CONSERVATION

We now consider the simplest electromagnetic extension suitable for the study of intense laser-plasma interactions.[5] We adopt the conventions of Ref. 5: we retain a single spatial dimension (the laser propagation direction), z, and two particle momenta: one in the direction of the laser polarization, x, and other in the propagation direction. Here, we retain the longitudinal component of the vector potential and do not otherwise impose a gauge-fixing condition. Although we consider the relativistic case, all of our results apply in the nonrelativistic limit. Adopting the appropriate generalization of (1) and following Ref. 5, the Lagrangian can be written as $\mathcal{L} = \mathcal{L}_P + \mathcal{L}_I + \mathcal{L}_F$, where

$$\mathcal{L}_P = -m_s c^2 \sum_{\alpha=1}^{N_p} w_\alpha \sqrt{1 - \frac{\dot{\xi}_x^{\alpha 2}}{c^2} - \frac{\dot{\xi}_z^{\alpha 2}}{c^2}}, \qquad (21a)$$

$$\mathcal{L}_I = q_s \sum_{\alpha=1}^{N_p} w_\alpha \sum_{i=1}^{N_g} \left(\frac{\dot{\xi}_x^\alpha}{c} A_{x,i} + \frac{\dot{\xi}_z^\alpha}{c} A_{z,i} - \varphi_i \right) \rho_i(\xi_z^\alpha), \quad (21b)$$

$$\mathcal{L}_F = \frac{\Delta z}{8\pi c^2} \sum_{i=1}^{N_g} (\dot{A}_{x,i}^2 + \dot{A}_{z,i}^2)$$
$$+ \frac{\Delta z}{8\pi} \sum_{i,j=1}^{N_g} \left(\frac{2}{c} \dot{A}_{z,i} \mathcal{D}_{ij} \varphi_j + A_{x,i} \mathcal{K}_{ij} A_{x,j} - \varphi_i \mathcal{K}_{ij} \varphi_j \right), \quad (21c)$$

where ξ_x^α and ξ_z^α are the x and z coordinates of the macroparticle positions, respectively, $A_{x,i}$ and $A_{z,i}$ are numerical approximations to $A_x(Z_i)$ and $A_z(Z_i)$, respectively, and $\mathcal{D}_{ij}$ and $\mathcal{K}_{ij}$ are central difference approximations to the first and second derivatives in z, respectively.

Consider a gauge transformation on the discretized potential[20] $A_{z,i} = A'_{z,i} + \sum_{k=1}^{N_g} \mathcal{D}_{ik} \Lambda_k$ and $\varphi_i = \varphi'_i - \dot{\Lambda}_i / c$. Certainly, in the continuous case, the action is invariant under this transformation. However, this does not imply invariance in the discrete case. Since the macro-particles are not directly involved in the transformation, we need only consider $\mathcal{L}_F$ and $\mathcal{L}_I$. From $\mathcal{L}_F$, we obtain the condition $\mathcal{K}_{ij} = \mathcal{D}_{ik} \mathcal{D}_{kj}$; while from $\mathcal{L}_I$, we have

$$\mathcal{L}_I = \mathcal{L}_I(A'_z, \varphi') + \frac{q_s}{c} \sum_{\alpha=1}^{N_p} w_\alpha \sum_{i=1}^{N_g} \frac{d}{dt} [\Lambda_i \rho_i(\xi_z^\alpha)]$$
$$- \frac{q_s}{c} \sum_{\alpha=1}^{N_p} w_\alpha \sum_{i=1}^{N_g} \Lambda_i \left(\sum_{k=1}^{N_g} \mathcal{D}_{ik} \rho_k + \frac{\partial \rho_i}{\partial \xi_z^\alpha} \right) \dot{\xi}_z^\alpha. \quad (22)$$

Gauge invariance requires the last term in (22) to vanish

$$\frac{\partial \rho_i}{\partial \xi_z^\alpha} + \mathcal{D}_{ik} \rho_k = 0. \qquad (23)$$

This is equivalent to

$$0 = q_s \frac{\partial \rho_i}{\partial \xi_z^\alpha} \dot{\xi}_z^\alpha + q_s \mathcal{D}_{ik} \rho_k \dot{\xi}_z^\alpha = q_s \frac{\partial \rho_i}{\partial t} + \mathcal{D}_{ik} \left(q_s \dot{\xi}_z^\alpha \rho_k \right)$$
$$= \frac{\partial \mathcal{N}_i}{\partial t} + \mathcal{D}_{ik} \mathcal{J}_{z,k}, \qquad (24)$$

where $\mathcal{N}_i$ and $\mathcal{J}_{z,i}$ are the numerical approximations at z_i to $\mathcal{N}$ and $\mathcal{J}_z$ [defined as in (2)], respectively.[21] It is straightforward to show that ρ_k defined by (7) cannot satisfy this condition. (This follows almost immediately from the fact that finite element basis functions are not everywhere differentiable.) The lack of an exact discrete analogue of the continuity equation is due to the fact that in the continuous case, the continuity equation is embedded within the reduction (1) and thus suffers from errors due to truncation when converted to discrete form.

Consider the average discrepancy in (23) as the macroparticle moves across a cell (ignoring the possible change in $\dot{\xi}_z^\alpha$)

$$\int_{x_i - \Delta x/2}^{x_i + \Delta x/2} d\xi \left[\frac{\partial \rho_i}{\partial \xi} + \sum_{k=1}^{N_g} \mathcal{D}_{ik} \rho_k(\xi) \right]$$
$$= \rho_i \Big|_{x_i - \Delta x/2}^{x_i + \Delta x/2} + \sum_{k=1}^{N_g} \mathcal{D}_{ik} \int_{x_i - \Delta x/2}^{x_i + \Delta x/2} d\xi \rho_k(\xi). \qquad (25)$$

Put $\xi = x_i + \Delta$, then from (7),

$$\rho_i(x_i + \Delta) = \int dx \, \Psi_i(x) \, S(x - x_i - \Delta)$$
$$= \int d\mu \, \Psi_i(x_i + \mu) \, S(\mu - \Delta). \qquad (26)$$

If Ψ_i is symmetric about $x = x_i$ (which is the case for linear and quadratic Lagrange elements), then $\Psi(x_i - \mu) = \Psi(x_i + \mu)$ and

$$\rho_i(x_i + \Delta) = \int d\mu \, \Psi_i(x_i - \mu) \, S(\mu - \Delta)$$
$$= \int d\mu \, \Psi_i(x_i + \mu) \, S(-\mu - \Delta). \qquad (27)$$

Further, if $S(x)$ is symmetric about $x = 0$, then

$$\rho_i(x_i + \Delta) = \int d\mu \, \Psi_i(x_i + \mu) \, S(\mu + \Delta) = \rho_i(x_i - \Delta) \quad (28)$$

and the first term on the right in (25) vanishes. The basis functions for linear and quadratic elements are simple replications of a fixed set of shapes with period one (linear) or period two (quadratic). As a result, $\Psi_{i+l}(x_i + \mu) = \Psi_{i-l}(x_i - \mu)$ for $l = 1, 2, \ldots$ and

$$\rho_{i+l}(x_i + \Delta) = \int d\mu \, \Psi_{i+l}(x_i + \mu) \, S(\mu - \Delta)$$

$$= \int d\mu \, \Psi_{i-l}(x_i - \mu) \, S(\mu - \Delta)$$

$$= \int d\mu \, \Psi_{i-l}(x_i + \mu) \, S(-\mu - \Delta)$$

$$= \int d\mu \, \Psi_{i-l}(x_i + \mu) \, S(\mu + \Delta)$$

$$= \rho_{i-l}(x_i - \Delta) \,, \tag{29}$$

leading to

$$\int_{x_i - \Delta x/2}^{x_i + \Delta x/2} d\xi \, \rho_{i+l}(\xi)$$

$$= \int_{-\Delta x/2}^{\Delta x/2} d\Delta \, \rho_{i+l}(x_i + \Delta) = \int_{-\Delta x/2}^{\Delta x/2} d\Delta \, \rho_{i+l}(x_i - \Delta)$$

$$= \int_{-\Delta x/2}^{\Delta x/2} d\Delta \, \rho_{i-l}(x_i + \Delta) = \int_{x_i - \Delta x/2}^{x_i + \Delta x/2} d\xi \, \rho_{i-l}(\xi) \,. \tag{30}$$

By assumption, $\mathcal{D}_{ik}$ is some central difference approximation to the first derivative and thus has the form

$$\mathcal{D}_{ik} = \sum_l \alpha_l (\delta_{i,k+l} - \delta_{i,k-l}). \tag{31}$$

Combining (30) and (31) gives

$$\sum_{k=1}^{N_g} \mathcal{D}_{ik} \int_{x_i - \Delta x/2}^{x_i + \Delta x/2} d\xi \, \rho_k(\xi)$$

$$= \sum_l \alpha_l \left[\int_{x_i - \Delta x/2}^{x_i + \Delta x/2} d\xi \, \rho_{i+l}(\xi) - \int_{x_i - \Delta x/2}^{x_i + \Delta x/2} d\xi \, \rho_{i-l}(\xi) \right] = 0 \tag{32}$$

and thus

$$\int_{x_i - \Delta x/2}^{x_i + \Delta x/2} d\xi \left[\frac{\partial \rho_i}{\partial \xi} + \sum_{i=1}^{N_g} \mathcal{D}_{ik} \, \rho_k(\xi) \right] = 0 \,. \tag{33}$$

Hence, as a macro-particle traverses a cell, provided the velocity is nearly constant, the discrepancy averages to zero. Thus, it is reasonable to expect that in a time-averaged sense, the condition for gauge invariance (also momentum and change conservation) is satisfied. Furthermore, this result is for a single macro-particle; as the number of macro-particles per cell increases, we expect the discrepancy in (23), when summed over all macro-particles in a cell (each of which is likely to be at a distinct location), to decrease.

From the Lagrangian (21), we obtain the equations of motion[5]

$$\dot{\pi}_x^\alpha = -\frac{q_s}{c} \frac{d}{dt} \sum_{k=1}^{N_g} A_{x,i} \, \rho_i(\xi_x^\alpha), \tag{34a}$$

$$\dot{\pi}_z^\alpha = -q_s \sum_{i=1}^{N_g} \left[\frac{1}{c} \dot{A}_{z,i} \, \rho_i(\xi_z^\alpha) + \left(\varphi_i - \frac{\dot{\xi}_x^\alpha}{c} A_{x,i} \right) \frac{\partial \rho_i}{\partial \xi_z^\alpha} \right], \tag{34b}$$

$$\sum_{j=1}^{N_g} \left(\mathcal{K}_{ij} \, \varphi_j + \frac{1}{c} \mathcal{D}_{ij} \dot{A}_{z,j} \right) = -\frac{4\pi q_s}{\Delta z} \sum_{\alpha=1}^{N_p} w_\alpha \, \rho_i(\xi_z^\alpha), \tag{34c}$$

$$\ddot{A}_{x,i} - c^2 \sum_{j=1}^{N_g} \mathcal{K}_{ij} A_{x,j} = \frac{4\pi q_s c}{\Delta z} \sum_{\alpha=1}^{N_p} w_\alpha \, \dot{\xi}_x^\alpha \, \rho_i(\xi_z^\alpha), \tag{34d}$$

$$\ddot{A}_{z,i} + c \sum_{j=1}^{N_g} \mathcal{D}_{ij} \dot{\varphi}_j = \frac{4\pi q_s c}{\Delta z} \sum_{\alpha=1}^{N_p} w_\alpha \, \dot{\xi}_z^\alpha \, \rho_i(\xi_z^\alpha), \tag{34e}$$

where $\pi_x^\alpha \equiv m_s \, \gamma_\alpha \, \dot{\xi}_x^\alpha$ and $\pi_z^\alpha \equiv m_s \, \gamma_\alpha \, \dot{\xi}_z^\alpha$ are the usual relativistic particle momenta with $\gamma_\alpha = \sqrt{m^2 c^2 + \pi_x^{\alpha 2} + \pi_z^{\alpha 2}}/mc$. The equation of motion for $\dot{\pi}_x^\alpha$, (34a), is just a statement of conservation of the momentum conjugate to a cyclic coordinate (ξ_x^α). Since our Lagrangian is time-independent, there is a conserved energy given by[5]

$$W = m_s c^2 \sum_{\alpha=1}^{N_p} w_\alpha \, \gamma_\alpha + \frac{\Delta z}{8\pi c^2} \sum_{i=1}^{N_g} \left(\dot{A}_{x,i}^2 + \dot{A}_{z,i}^2 \right)$$

$$- \frac{\Delta z}{8\pi} \sum_{i,j=1}^{N_g} \left(\varphi_i K_{ij} \varphi_j + A_i K_{ij} A_j - \frac{2}{c} \dot{A}_{z,i} \, \mathcal{D}_{ij} \, \varphi_j \right). \tag{35}$$

The remaining conservation law from the continuous system (assuming the system is unbounded) is momentum conservation. The components of the total momentum (particle plus fields) are

$$P_x = \sum_{\alpha=1}^{N_p} w_\alpha \, \pi_x^\alpha - \frac{\Delta z}{4\pi c} \sum_{i,j=1}^{N_g} \dot{A}_{x,i} \, \mathcal{D}_{ij} \left(\frac{1}{c} \dot{A}_{z,j} + \sum_{k=1}^{N_g} \mathcal{D}_{jk} \, \varphi_k \right), \tag{36a}$$

$$P_z = \sum_{\alpha=1}^{N_p} w_\alpha \, \pi_z^\alpha - \frac{\Delta z}{4\pi c^2} \sum_{i,j=1}^{N_g} \dot{A}_{x,i} \, \mathcal{D}_{ij} \, A_{x,j} \,. \tag{36b}$$

First consider P_z. A long calculation yields

$$\dot{P}_z = -\frac{\Delta z}{4\pi q_s c} \sum_{i,j=1}^{N_g} \dot{A}_{z,i} \left(\mathcal{K}_{ij} - \sum_{l=1}^{N_g} \mathcal{D}_{il} \mathcal{D}_{lj} \right) \varphi_j$$

$$- q_s \sum_{i=1}^{N_g} \sum_{\alpha=1}^{N_p} w_\alpha \left(\varphi_i - A_{x,i} \frac{\dot{\xi}_x^\alpha}{c} \right) \left(\frac{\partial \rho_k}{\partial \xi_z^\alpha} - \sum_{j=1}^{N_g} \mathcal{D}_{ij} \rho_j \right)$$

$$- \frac{\Delta z}{4\pi q_s} \sum_{i,j=1}^{N_g} \left[\varphi_i (\mathcal{K}\mathcal{D})_{ij} \varphi_j + A_{x,i} (\mathcal{K}\mathcal{D})_{ij} A_{x,j} \right]. \tag{37}$$

If we take $\mathcal{K} = \mathcal{D}^2$ (as required for $\mathcal{L}_F$ to be gauge invariant), then $\mathcal{K}\mathcal{D} = \mathcal{D}^3$ is antisymmetric and terms of the form $\sum_{i,j=1}^{N_g} a_i (\mathcal{K}\mathcal{D})_{ij} a_j = \sum_{i,j=1}^{N_g} a_i (\mathcal{D}\mathcal{D}\mathcal{D})_{ij} a_j$ vanish. Using these results, (37) becomes

$$\dot{P}_z = -q_s \sum_{i=1}^{N_g} \sum_{\alpha=1}^{N_p} w_\alpha \left(\varphi_i - A_{x,i} \frac{\dot{\xi}_x^\alpha}{c} \right) \left(\frac{\partial \rho_k}{\partial \xi_z^\alpha} + \sum_{j=1}^{N_g} \mathcal{D}_{ij} \rho_j \right). \tag{38}$$

We see that (23) is also required for momentum conservation. While this cannot be achieved exactly in the presence of a spatial grid, we expect that on average momentum will be well conserved by the arguments leading to (33). In the electrostatic case, it is straightforward to show that this condition is also required for exact momentum conservation. From P_x we find, with $\mathcal{K} = \mathcal{D}^2$,

$$\dot{P}_x = -\frac{q_s}{c}\sum_{\alpha=1}^{N_p} w_\alpha\, \dot{\xi}_z^\alpha \sum_{i=1}^{N_g} A_{x,i}\left(\frac{\partial \rho_i}{\partial \xi_z^\alpha} + \sum_{j=1}^{N_g}\mathcal{D}_{ij}\,\rho_j\right), \quad (39)$$

which has the same form as (38). Thus even though we have exact translation invariance in the x-direction, the continuity equation is still required for momentum conservation.

As is well known, the connection between Gauss' and Ampere's Laws also involves the continuity equation. Consider Gauss' Law with the assumption that $\mathcal{K} = \mathcal{D}^2$. In this case, we can write (34c) as

$$\sum_{j=1}^{N_g}\mathcal{D}_{ij}\left(\sum_{k=1}^{N_g}\mathcal{D}_{jk}\,\varphi_k + \frac{1}{c}\dot{A}_{z,j}\right) = -\frac{4\pi q_s}{\Delta z}\sum_{\alpha=1}^{N_p} w_\alpha \rho_i(\xi_z^\alpha). \quad (40)$$

Differentiating with respect to time and multiplying by $c\,\mathcal{D}^{-1}$ gives

$$\ddot{A}_{z,j} + c\sum_{k=1}^{N_g}\mathcal{D}_{jk}\,\dot{\varphi}_k$$

$$= \frac{4\pi q_s c}{\Delta z}\sum_{\alpha=1}^{N_p} w_\alpha\,\dot{\xi}_z^\alpha\,\rho_j - \frac{4\pi q_s c}{\Delta z}\sum_{i=1}^{N_g}\mathcal{D}_{ji}^{-1}$$

$$\times \sum_{\alpha=1}^{N_p} w_\alpha\,\dot{\xi}_z^\alpha\left(\frac{\partial \rho_i}{\partial \xi_z^\alpha} + \sum_{k=1}^{N_g}\mathcal{D}_{ik}\,\rho_k\right). \quad (41)$$

Thus we see that Gauss's Law and the z-component of Ampere's Law are only consistent to the extent that

$$\frac{\partial \rho_i}{\partial \xi_z^\alpha} + \sum_{k=1}^{N_g}\mathcal{D}_{ik}\,\rho_k \quad (42)$$

vanishes. This is the same condition, (23), required for gauge invariance.

As we have seen, gauge invariance and momentum conservation all hinge on the discrete form of the continuity equation, (23). Using finite elements for interpolation (in this context, it is immaterial whether finite elements or finite differences are used to evaluate $\mathcal{L}_F$), we have seen that this condition is only satisfied on average. Following Ref. 1, we now consider a general discrete spatial representation using a truncated basis. Let $\Phi_m(x)$, $m = 1, 2, \ldots, M$ be the first M elements of a complete basis. Clearly, we cannot expect to expand arbitrary functions with this collection of basis elements as that would necessarily require completeness. Instead, consider a mapping from functions $f(x)$ to

$$\hat{f}(x) = \sum_{m=1}^{M} f_m \Phi_m(x), \quad (43)$$

with

$$f_m = \int dx\, f(x)\, \Phi_m^\dagger(x), \quad (44)$$

where $\Phi_k^\dagger(x)$ is the dual to $\Phi_k(x)$ and satisfies

$$\int dx\, \Phi_i(x)\, \Phi_j^\dagger(x) = \delta_{ij}. \quad (45)$$

This mapping is a projection and provides a discrete representation, f_m, for any $f(x)$. (Since it is a projection, many functions may have the same discrete representation.) Let

$$\varrho(x) = \sum_{m=1}^{M}\varrho_m\, \Phi_m(x) \quad (46)$$

and

$$\varrho_m = \int dx\, S(x - \xi_\alpha)\, \Phi_m^\dagger(x), \quad (47)$$

i.e, $\varrho(x)$ is the projection of $S(x - \xi_\alpha)$. For $\varrho(x)$ to satisfy the continuity equation, the projection must preserve $\partial S/\partial x = -\partial S/\partial \xi_\alpha$, thus we require $\partial \varrho/\partial x = -\partial \varrho/\partial \xi_\alpha$. If our basis was complete, this property would be automatic, otherwise this condition implies a significant restriction on $\Phi_m(x)$. Now

$$\frac{\partial \varrho}{\partial \xi_\alpha} = \sum_{m=1}^{M}\frac{\partial \varrho_m}{\partial \xi_\alpha}\Phi_m(x)$$

$$= \sum_{m=1}^{M}\Phi_m(x)\int dx'\,\frac{\partial S(x' - \xi_\alpha)}{\partial \xi_\alpha}\,\Phi_m^\dagger(x')$$

$$= -\sum_{m=1}^{M}\Phi_m(x)\int dx'\,\frac{\partial S(x' - \xi_\alpha)}{\partial x'}\,\Phi_m^\dagger(x')$$

$$= \sum_{m=1}^{M}\Phi_m(x)\int dx'\, S(x' - \xi_\alpha)\,\frac{d\Phi_m^\dagger(x')}{dx'} \quad (48)$$

and

$$\frac{\partial \varrho}{\partial x} = \sum_{m=1}^{M}\varrho_m\,\frac{d\Phi_m(x)}{dx}. \quad (49)$$

Thus, our requirement on ϱ implies

$$\sum_{m=1}^{M}\frac{d\Phi_m(x)}{dx}\int dx'\, S(x' - \xi_\alpha)\,\Phi_m^\dagger(x')$$

$$= -\sum_{m=1}^{M}\Phi_m(x)\int dx'\, S(x' - \xi_\alpha)\,\frac{d\Phi_m^\dagger(x')}{dx'}, \quad (50)$$

which must hold for any S. This is equivalent to the condition found in Ref. 1 for the Lagrangian to be translation invariant [see (55) therein]. Since translation invariance implies momentum conservation and momentum

conservation, in turn, relies on charge conservation, it is reasonable that the condition for translation invariance should be the selfsame condition for the continuity equation to be exactly satisfied.

Consider any $f(x)$ and assume (50) holds. Then,

$$
\begin{aligned}
\frac{d\hat{f}}{dx} &= \sum_{m=1}^{M} \frac{d\Phi_m(x)}{dx} \int dx' f(x') \, \Phi_m^\dagger(x') \\
&= -\sum_{m=1}^{M} \Phi_m(x) \int dx' f(x') \frac{d\Phi_m^\dagger(x')}{dx'} \\
&= \sum_{m=1}^{M} \Phi_m(x) \int dx' \frac{df(x')}{dx'} \, \Phi_m^\dagger(x') \,.
\end{aligned}
\tag{51}
$$

Thus, we see that (50) implies that the spatial derivative commutes with the projection, i.e., if $g(x) = df(x)/dx$, then $\hat{g}(x) = d\hat{f}(x)/dx$. Equivalently, the basis must be such that the derivative operation is represented exactly under the projection (43). For finite elements, this is simply not the case, explaining the failure of (23) to hold.

Since (50) must hold for any S, in particular, it must be true that

$$
\begin{aligned}
\sum_{m=1}^{M} \frac{d\Phi_m(x)}{dx} &\int dx' \Phi_n(x') \, \Phi_m^\dagger(x') \\
&= -\sum_{m=1}^{M} \Phi_m(x) \int dx' \Phi_n(x') \frac{d\Phi_m^\dagger(x')}{dx'} \,.
\end{aligned}
\tag{52}
$$

With (45), this becomes

$$
\begin{aligned}
\frac{d\Phi_n(x)}{dx} &= -\sum_{m=1}^{M} \Phi_m(x) \int dx' \, \Phi_n(x') \frac{d\Phi_m^\dagger(x')}{dx'} \\
&= \sum_{m=1}^{M} \Phi_m(x) \int dx' \, \Phi_m^\dagger(x') \frac{d\Phi_n(x')}{dx'} \\
&= \mathcal{D}_{mn} \, \Phi_m(x) \,,
\end{aligned}
\tag{53}
$$

where

$$
\mathcal{D}_{ij} = \int dx \, \Phi_i^\dagger(x) \frac{d\Phi_j(x)}{dx} \,,
\tag{54}
$$

is the discrete representation of the derivative, viz., if $g(x) = df(x)/dx$, then $g_n = \sum_{m=1}^{M} \mathcal{D}_{nm} f_m$. Now

$$
\frac{\partial \varrho}{\partial x} = \sum_{m=1}^{M} \varrho_m \frac{\Phi_m(x)}{dx} = \sum_{n,m=1}^{M} \mathcal{D}_{mn} \, \varrho_n \, \Phi_m(x),
\tag{55}
$$

while

$$
\frac{\partial \varrho}{\partial \xi_\alpha} = \sum_{m=1}^{M} \frac{\partial \varrho_m}{\partial \xi_\alpha} \Phi_m(x) \,.
\tag{56}
$$

Our requirement on ϱ can now be expressed as

$$
\frac{\partial \varrho_m}{\partial \xi_\alpha} + \sum_{n=1}^{M} \mathcal{D}_{mn} \, \varrho_n = 0,
\tag{57}
$$

which is exactly the condition require for gauge invariance and momentum conservation.

It appears that the only way to satisfy (50) is for Φ_m to be a truncated Fourier basis.[1] Thus, using a Fourier representation of the fields, we expect the macro-particle model will have exact gauge invariance as well as charge and momentum conservation. Computationally, the Fourier representation appears to be sufficiently expensive compared to the finite-difference representation such as to be unsuitable for production work. Nonetheless, it is valuable as a benchmarking tool to assess the consequences of the approximate conservation laws in the finite-difference case.

V. CONCLUSIONS

We have reviewed a recent variational formulation of macro-particle methods. For the one-dimensional electrostatic case, we have considered both a standard second order integrator as well as a second-order symplectic integrator. For the problem of weak Landau damping, the symplectic integrator yielded acceptably accurate results with a considerably larger time-step than did the standard integrator, leading to a significant advantage in computational efficiency for the symplectic integrator. We compared the macro-particle solutions to a well-converged solution of the Vlasov–Poisson equation, finding surprisingly good agreement. For the problem considered, even the symplectic method requires significantly more computational effort than does the Eulerian solver. Ultimately, phase-space must be fully resolved and the Eulerian method appears to have the advantage. (Of course, this advantage fades quickly as the dimension of phase-space increases.) Both macro-particle methods, despite being initialized with thermal distributions, yielded solutions low in numerical noise. We analysed an implicit time-integrator and showed this method exactly conserved energy in both the nonrelativistic and relativistic cases. Exact energy conservation required the use of fields rather than potentials and thus relies on a noncanonical Hamiltonian formulation of the macro-particle model.

We have examined the simplest electromagnetic extension and considered in detail the affects of spatial discretization on the continuity equation. We have found when using finite elements to interpolate the potential between the grid points, it is not possible to exactly conserve charge, resulting in departures from exact gauge invariance and momentum conservation. We examined these errors and showed they average to zero as the macro-particle moves across the cell (assuming small changes in the macro-particle velocity during the transversal). These results also suggest that such errors can be reduced by using sufficient macro-particles per cell. We showed exact charge conservation is possible when using a truncated basis for the spatial representation. We derived conditions the basis must satisfy to ensure charge conservation and showed these conditions amounted to the requirement that the basis exactly represent spatial derivatives. Although these results were obtained in one spatial dimension, they readily extent to three dimensions assuming a Cartesian product of one-dimensional finite elements are used for interpolation. No further assumptions appear

necessary to extent the truncated Fourier basis representation to three dimensions. The Fourier-based method uses the same reduction as the gridded methods and therefore offers the opportunity to carefully assess the effects of the approximate conservation laws in the gridded case. It appears straightforward to perform the Legendre transformation, with either the Fourier or gridded representations, yielding a canonical Hamiltonian system for macro-particles and fields, which opens the possibility of using symplectic integration on the combined macro-particle field phase-space.

ACKNOWLEDGMENTS

[1]E. G. Evstatiev and B. A. Shadwick, J. Comput. Phys. **245**, 376 (2013).

[2]J. M. Dawson, Rev. Mod. Phys. **55**, 403 (1983).

[3]C. K. Birdsall and A. B. Langdon, *Plasma Physics via Computer Simulations, Plasma Physics Series* (Institute of Physics Publishing, Bristol, 1991).

[4]R. W. Hockney and J. W. Eastwood, *Computer Simulation Using Particles* (Taylor & Francis Group, New York, 1988).

[5]A. B. Stamm, B. A. Shadwick, and E. G. Evstatiev, "Variational formulation of macro-particle models for electromagnetic plasma simulations," IEEE Trans. Plasma Sci. (to be published).

[6]F. E. Low, Proc. R. Soc. London, Ser. A **248**, 282 (1958).

[7]Formally, there is no need to approximate the field energy using the same finite elements as used for the interpolation, but there seems little to be gained from exploiting this freedom.

[8]J. E. Marsden and M. West, Acta Numer. **10**, 357 (2001).

[9]J. Reyes and B. Shadwick, in *2013 19th IEEE Pulsed Power Conference* (2013), pp. 1–5.

[10]P. J. Channell and C. Scovel, Nonlinearity **3**, 231 (1990).

[11]L. Verlet, Phys. Rev. **159**, 98 (1967).

[12]E. Hairer, C. Lubich, and G. Wanner, *Geometric Numerical Integration: Structure-Preserving Algorithms for Ordinary Differential Equations*, Springer Series in Computational Mathematics (Springer, 2010).

[13]N. A. Krall and A. W. Trivelpiece, *Principles of Plasma Physics* (McGraw-Hill, New York, 1973).

[14]In this problem, it would be natural to use variable-weight macro-particles to more efficiently represent the tail of the distribution. Here, our interest is in understanding the sensitivity of the solution to errors in phase space, which we expect should not be qualitatively different in the case of fixed-weight macro-particles.

[15]M. Carrié and B. A. Shadwick, "An implicit solver for the Vlasov–Poisson equation," Bull. Am. Phys. Soc. **57**(12) (2012); available at http://meetings.aps.org/link/BAPS.2012.DPP.UP8.22.

[16]S. Markidis and G. Lapenta, J. Comput. Phys. **230**, 7037 (2011).

[17]G. Chen, L. Chacón, and D. Barnes, J. Comput. Phys. **230**, 7018 (2011).

[18]B. A. Shadwick, J. C. Bowman, and P. J. Morrison, SIAM J. Appl. Math **59**, 1112 (1998).

[19]J. Isaac, private communication (2012).

[20]Due to our geometry, only A_z has a non-trivial gauge transformation.

[21]The wave equation for the longitudinal vector potential is consistent with this definition of the current density.