Accelerated multiboson algorithm for Coulomb gases with dynamical dielectric effects

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(Received 8 March 2006; published 29 June 2006)

A recent reformulation [Phys. Rev. E **73**, 016705 (2006)] of the problem of Coulomb gases in the presence of a dynamical dielectric medium showed that finite-temperature simulations of such systems can be accomplished on the basis of completely local Hamiltonians on a spatial lattice by including additional bosonic fields. For large systems, the Monte Carlo algorithm proposed in the above-cited work becomes inefficient due to a low acceptance rate for particle moves in a fixed background multiboson field. We show here how this problem can be circumvented by use of a coupled particle-multiboson update procedure that improves acceptance rates on large lattices by orders of magnitude. The method is tested on a one-component plasma with neutral dielectric particles for a variety of system sizes.

DOI: 10.1103/PhysRevE.73.066711 PACS number(s): 05.10.−a, 61.20.Ja, 61.20.Qg, 05.50.+q

I. INTRODUCTION

Some years ago, Maggs and Rossetto[1] introduced a local reformulation of the statistical mechanics of a Coulomb gas of mobile charged entities, relying on the fact that the long-range Coulomb interaction could be recovered from a Hamiltonian written in terms of an electric field variable coupled to the charge density via Gauss's law. Since the publication of this paper, more recent work has focused on improving the efficiency and capability of the method so that it may be applied to larger and more realistic systems [2–6]. The partition function in this approach is written as a functional integral over an electric field variable containing a physical longitudinal (gradient) part incorporating the electrostatic potential energy, as well as an unphysical transverse (curl) part. The latter component of the electric field can easily be seen to decouple from the charged particle motion, provided the dielectric constant does not change in the course of the simulation (i.e., is nondynamical). Note that a spatially varying dielectric medium is perfectly allowable in the context of the original method: the integration over the transverse parts of the electric field variable only introduces spurious interactions if the dielectric function is also a function of the particle locations. This latter situation is of course quite common in simulations of biophysical interest, for example if the charges are attached to a polymer undergoing conformational changes.

In a recent paper [7], we suggested a new algorithm for compensating for the spurious interactions introduced by the integration over the curl part of the electric field in situations of this type. The extra terms actually correspond simply to the inverse determinant of the Poisson operator $\vec{\nabla}\cdot[\epsilon(\vec{r})\vec{\nabla}]$. Removing them therefore amounts to the problem of introducing a positive power of the determinant of a local operator into a functional integral. This problem has been intensively studied in elementary particle theory, where the inclusion of virtual quark effects in lattice quantum chromodynamics simulations requires the introduction of just such a determinant in a functional integral. In particular, the multiboson method introduced by Lüscher [8] seems ideally suited for the task at hand, for reasons explained below. Re-expressing the Poisson determinant in terms of an integral over a finite number N_B of additional bosonic fields, we arrive at a local Hamiltonian and a partition function that can be easily simulated by standard Metropolis or heatbath techniques. In this approach, an update of the system proceeds by successive, and independent, updates of (a) charged particle locations, (b) electric field values (on the links of the lattice), and (c) all N_B multiboson fields (on the sites of the lattice).

The algorithm studied in Ref. [7] does suffer, however, from a serious drawback. The multiboson fields are in general rather strongly coupled to the particle locations, so that a particle move leaving the boson fields unchanged becomes difficult when it induces a large corresponding change in the multiboson energy, without allowing the multiboson fields to relax in response to the new particle location. The problem becomes acute when the number N_B of multiboson fields is increased: for example, to model more accurately the low momentum modes on a large lattice. One then finds an acceptance rate for particle moves that decreases exponentially with N_B. The goal of the present paper is to show that a modified update procedure which couples particle moves and boson field updates greatly ameliorates this acceptance problem. Efficient simulation with a large number of multiboson fields is necessary for performing realistic simulations on large lattices.

In Sec. II, we review the basic multiboson algorithm introduced in Ref. [7], valid for systems with dynamically varying dielectric functions. The coupled update method, allowing the multiboson fields to relax appropriately as the particles are moved, is explained in detail in Sec. III. Detailed numerical tests of the method, with comparisons to the original, uncoupled approach, are presented in Sec. IV. Finally, we offer some concluding remarks in Sec. V.

II. MULTIBOSON FORMULATION OF COULOMB GAS SYSTEMS WITH VARYING DIELECTRIC EFFECTS

In this section we review the multiboson reformulation of Ref. [7] for Coulomb gas systems with varying dielectric effects. Consider the partition function of a system consisting

of N free charges (mobile or fixed) e_i at locations $\vec{r}_i$, corresponding to a free charge density

$$\rho(\vec{r}) = \sum_i e_i \delta(\vec{r} - \vec{r}_i) \tag{1}$$

where the system is also described by a linear dielectric function (here assumed isotropic) $\epsilon(\vec{r})$. We shall suppress the dependence of $\epsilon(\vec{r})$ on particle locations, but the procedure we shall describe is precisely devised to properly account for this dependence in the electrostatic energetics of the problem. Breaking the electric displacement into longitudinal and transverse parts using the general Helmholtz decomposition,

$$\vec{D}(\vec{r}) = -\epsilon(\vec{r})\vec{\nabla}\phi(\vec{r}) + \vec{\nabla} \times \vec{A}(\vec{r}) \tag{2}$$

$$= \vec{D}^{\parallel}(\vec{r}) + \vec{D}^{\mathrm{tr}}(\vec{r}). \tag{3}$$

As the transverse and longitudinal components are orthogonal to each other, one has

$$\int d\vec{r} \frac{\vec{D}^2}{\epsilon(\vec{r})} = \int d\vec{r} \frac{\vec{D}^{\parallel}(\vec{r})^2}{\epsilon(\vec{r})} + \int d\vec{r} \frac{\vec{D}^{\mathrm{tr}}(\vec{r})^2}{\epsilon(\vec{r})}. \tag{4}$$

It follows that the imposition of Maxwell's second law (curl-free electric field) implies that the electrostatic energy of the system is given purely in terms of the longitudinal part of the electric displacement,

$$H_{\mathrm{es}} = \frac{1}{2} \int d\vec{r} \frac{\vec{D}^{\parallel}(\vec{r})^2}{\epsilon(\vec{r})}. \tag{5}$$

Accordingly, the canonical partition function for the system at inverse temperature β becomes

$$Z = \int \prod_{i=1}^{N} d\vec{r}_i e^{-\beta H_{\mathrm{es}}}, \tag{6}$$

where $\vec{D}^{\parallel}$ must be determined by first solving $-\vec{\nabla}\cdot(\epsilon\vec{\nabla}\phi) = \rho$, from which one obtains $\vec{D}^{\parallel} = -\epsilon(\vec{r})\vec{\nabla}\phi(\vec{r})$. Note that the (nonexistent) transverse part of the displacement field plays no role in this result.

In Ref. [7] we have shown how to write a representation for the above partition function by writing the Coulomb energy Boltzmann weight $e^{-\beta H_{\mathrm{es}}}$ in terms of an integral over an unrestricted electric displacement field $\vec{D}(\vec{r})$ (i.e., one containing both longitudinal and transverse parts), as well as over a set of multiboson fields with a local Hamiltonian. The integration over the multiboson fields is arranged to generate a factor that exactly cancels the contribution from the integral over the spurious transverse part $\vec{D}^{\mathrm{tr}}(\vec{r})$ for arbitrary dielectric functions $\epsilon(\vec{r})$. Although the factor itself is a determinant and highly nonlocal, the multiboson Hamiltonian is local and therefore conventional Monte Carlo simulation techniques can be applied.

First, we review some notational issues (for further details, see [7]). In order to write a well-defined functional integral for Z, we consider a lattice Coulomb gas with an electric displacement vector field $D_{n\mu}$ defined on lattice links, where lattice sites are denoted n and $\mu = 1, 2, 3$ indicating the spatial direction of the link. Dielectric values are associated with links on the lattice (rather than sites) so that the dielectric function on the lattice becomes $\epsilon_{n\mu}$. Introducing left (right) lattice derivatives $\bar{\Delta}$ (Δ), the lattice version of Eq. (2) becomes

$$D_{n\mu} = D^{\parallel}_{n\mu} + D^{\mathrm{tr}}_{n\mu} \tag{7}$$

$$= -\epsilon_{n\mu}\Delta_\mu \phi_n + \sum_{\nu\sigma} \epsilon_{\mu\nu\sigma} \bar{\Delta}_\nu A_{n\sigma}. \tag{8}$$

Here the electrostatic potential is represented by a lattice site field ϕ_n satisfying the Poisson equation

$$-\sum_\mu \bar{\Delta}_\mu (\epsilon_{n\mu}\Delta_\mu \phi_n) = \rho_n, \tag{9}$$

$$\rho_n = \sum_i e_i \delta_{n r_i}. \tag{10}$$

It is then straightforward to show that the contribution to the functional integral

$$Z' \equiv \int \prod_{n\mu} dD_{n\mu} \exp\left(-\frac{\beta}{2} \sum_{n\mu} D^2_{n\mu} \right) \tag{11}$$

from the integration over the unphysical transverse degrees of freedom $D^{\mathrm{tr}}_{n\mu}$ yields the factor $(\Pi_{n\mu}\sqrt{\epsilon_{n\mu}})\det^{-1/2}(\mathcal{M})$, where $\mathcal{M}$ is essentially the lattice Poisson operator:

$$\mathcal{M}\lambda_n \equiv \left(-\sum_\mu \bar{\Delta}_\mu \epsilon_\mu \Delta_\mu \right)\lambda_n = \sum_{i=1}^{6} \epsilon_{ni}\lambda_n - \sum_{i=1}^{6} \epsilon_{ni}\lambda_{n+i}. \tag{12}$$

The unwanted determinant factor induced by the transverse integrations can be removed by introducing a set of additional fields with a local Hamiltonian chosen to generate a *positive* square-root determinant canceling the unwanted contribution. As explained in [7], one begins from a uniform polynomial approximation to the function $1/s$ in the interval $[\delta, 1]$ for small δ. In terms of the complex roots of the polynomial $z_k = \mu_k + i\nu_k$, one may choose, for example (the choice is not unique and partly a matter of convenience [8]), the Chebyshev polynomial of order $2N_B$ with

$$\frac{1}{s} \simeq P(s) \equiv C \prod_{k=1}^{N_B} [(s - \mu_k)^2 + \nu_k^2], \tag{13}$$

$$\mu_k = \frac{1}{2}(1 + \delta)\left(1 - \cos \frac{2\pi k}{2N_B + 1} \right), \tag{14}$$

$$\nu_k = \sqrt{\delta} \sin \frac{2\pi k}{2N_B + 1}. \tag{15}$$

This representation extends as follows to the determinant of a real positive symmetric operator with spectrum in the interval $[0,1]$:

$$\det^{+1/2}(\mathcal{M}) \simeq \prod_{k=1}^{N_B} \det^{-1/2}[(\mathcal{M}-\mu_k)^2+\nu_k^2] \tag{16}$$

where the representation becomes exact in the limit $N_B \to \infty$, $\delta \to 0$. (In practice, the Poisson operator needs to be rescaled, so that its spectrum fits in the unit interval.) The crucial step in the multiboson procedure is the replacement of the determinant factor in Eq. (16) by an equivalent Gaussian integral over a set of N_B boson site fields $\phi_n^{(k)}$, $k=1,2,\ldots N_B$. The choice of N_B is dictated by the necessity to adequately describe the low eigenvalues of the Poisson operator $\mathcal{M}$: in Ref. [7], this was determined empirically by studying a model in which the structure factor of the system was analytically known in the charge-free limit. More generally, we expect that as the lowest eigenvalue of $\mathcal{M}$ on a lattice of dimension $L\times L\times L$ is typically of order $1/L^2$, the value of N_B will have to increase as the lattice size does. However, the precise character of the scaling of N_B with L clearly depends on the sensitivity of the observables studied to the infrared spectrum of $\mathcal{M}$.

Inserting a δ function to enforce the lattice version of Gauss's law (thereby fixing the longitudinal part of the electric displacement appropriately), the expression found for the correct partition function (Eq.(6)) [7] becomes

$$\begin{aligned} Z = \int \prod_i d\vec{r}_i \prod_{n\mu} dD_{n\mu} \prod_{kn} d\phi_n^{(k)} \delta\left(\sum_\mu \bar{\Delta}_\mu D_{n\mu} - \rho_n\right) \\ \times \exp\left(-\frac{1}{2}\sum_{n\mu} \ln(\epsilon_{n\mu})\right) \exp\left(-\frac{\beta}{2}\sum_{n\mu} D_{n\mu}^2/\epsilon_{n\mu}\right) \\ \times \exp\left(-\sum_{k=1}^{N_B} \phi^{(k)}[(\mathcal{M}-\mu_k)^2+\nu_k^2]\phi^{(k)}\right). \end{aligned} \tag{17}$$

Note that the effective Hamiltonian appearing in the exponential here is completely local. Monte Carlo simulation of the system is in principle straightforward: a state of the system is characterized by (i) particle locations $\vec{r}_i$, which in general will influence the dielectric function $\epsilon(\vec{r})$ [which more accurately should be denoted $\epsilon(\vec{r};\vec{r}_i)$], (ii) the lattice displacement field $D_{n\mu}$ (respecting locally the Gauss's law constraint), and (iii) the N_B auxiliary scalar fields $\phi^{(k)}$, and simulation requires updates of all of these variables with a procedure respecting detailed balance and according to the indicated Boltzmann weight.

III. EFFICIENT MONTE CARLO PROCEDURE FOR A COULOMB GAS–MULTIBOSON SYSTEM

In [7], the multiboson approach was tested on a system of particles (both neutral and charged) with a dielectric constant different from that of the ambient medium. This model, first studied in Ref. [2], provides a clean testbed for algorithms dealing with the full electrostatic energetics of a system with a dynamical dielectric function. The latter changes through the simulation as the dielectric constant along a link in the μ direction from a lattice site n is defined through the relation

$$\frac{2}{\epsilon_{n\mu}} = \frac{1}{\epsilon_n} + \frac{1}{\epsilon_{n+\mu}}, \tag{18}$$

where ϵ_n and $\epsilon_{n+\mu}$ are either the background dielectric constant or the particle dielectric constant depending on whether there is a particle on site n or site $n+\mu$, respectively. For example, in the simulations discussed below, the background dielectric constant is set to 1.0, while the dielectric constant associated with the particle is set to 0.05. If the particles are electrically neutral, then we expect the electric displacement to vanish irrespective of the particle locations, leading to a flat (wave-number independent) density-density structure factor. Reference [7] shows that simulations of Eq. (17) with a relatively small number of multiboson fields ($N_B=4$ on a $16\times16\times16$ lattice) the neutral system yields a flat structure factor within statistical errors. For the rest of this paper, we shall use this model system to discuss issues of acceptance rates and simulation efficiency in the multiboson approach.

Unfortunately, the simulation procedure of Ref. [7], which we now review briefly, leads to an acceptance rate for particle moves that falls extremely rapidly as the number of multiboson fields is increased. For example, in our $16\times16\times16$ test lattice the procedure of Ref. [7] gives a particle move acceptance rate of 0.011 when eight multiboson fields are used, but the acceptance rate drops to less than 2×10^{-7} when 32 multiboson fields are used. As we emphasized above, increasing N_B will be necessary if we wish to go to much larger lattices, in order to apply the method to systems of real biophysical interest, for example. Specifically, the Monte Carlo procedure of [7] consisted of (1) a Metropolis move of a particle (randomly chosen) to a neighboring site, holding the electric displacement field $D_{n\mu}$ and the multiboson fields $\phi_n^{(k)}$ fixed; (2) a heat-bath (or worm [9]) update of the electric displacement field $D_{n\mu}$, with particle locations and multiboson fields held fixed; and (3) a Metropolis (or heat-bath) update of the multiboson fields, with electric displacement field and particle locations held fixed.

The acceptance problems of the method arise from the first step: Metropolis moves of the particles along lattice links. As the number of multiboson fields increases, the change in the contribution of the multiboson Hamiltonian to the Boltzmann weight increases (roughly linearly in N_B) and the acceptance rate for moves decreases exponentially. The origin of the decrease is simply that the displacement of a particle to a neighboring site leaving the multiboson fields unchanged places the system on the tail of the old multiboson Gaussian, with the multiboson Gaussian corresponding to the new particle location having very little overlap with the old one. The heat-bath approaches used in the second and third steps above have of course no such acceptance problems.

The displacement of the multiboson Gaussian induced by a particle move holds the key to finding a more efficient move algorithm: one clearly needs to update the particle positions and multiboson fields simultaneously. We now show that the Gaussian dependence of the Hamiltonian on the multiboson fields allows us to do this with a heat-bath approach that yields greatly increased (for larger values of N_B, by several orders of magnitude) acceptance rates for particle

moves. Let us denote the multiboson contribution to the Boltzmann weight in Eq. (17) by $e^{-S_{\rm mbos}}$. Now consider a particle move across a link connecting two nearest-neighbor sites a, b on the lattice (i.e., we assume that initially there is a particle at one but not both of these sites). The complete set of multiboson fields on the lattice can be grouped as $(\phi_a^i, \phi_b^i, \phi'^i)$, $i=1,2,\ldots,N_B$, where the fields *not* on sites a or b are collectively labeled ϕ'. The next step is to expose the dependence of the multiboson energy on just the fields at sites a and b: this will allow us to derive a heat-bath procedure for simultaneously moving the particle between a and b and updating all multiboson fields on these two sites, thereby "adapting" the multiboson fields dynamically to the updated particle position. As the multiboson energy is a quadratic function of the multiboson fields, we must have

$$S_{\rm mbos} = \sum_{i=1}^{N_B} [A_i(\phi_a^i)^2 + B_i(\phi_b^i)^2 + 2G_i\phi_a^i\phi_b^i + C_i\phi_a^i + D_i\phi_b^i] + S_{\text{non-}ab}(\phi', \epsilon). \tag{19}$$

Here, the coefficients A_i, B_i, G_i, C_i, D_i, as well as the residual term $S_{\text{non-}ab}$ all depend on the fields ϕ' not on the pair of sites a, b, as well as the dielectric field ϵ, which of course depends on particle locations via Eq. (18). It is straightforward to find explicit expressions for these coefficients in terms of ϵ and the ϕ' fields. We shall use Greek indices $\rho,\sigma,\tau,\ldots$, running over six values, to denote positive and negative spatial directions out of a given lattice site, while unit vectors in the corresponding directions are denoted $\hat{\rho}$, etc. Now let us assume that site b is the nearest neighbor of site a in the σ direction. Defining the site field

$$E_n \equiv \sum_\rho \epsilon_{n\rho} \tag{20}$$

one finds for the quadratic coefficients

$$A_i = (E_a - \mu_i)^2 + \sum_\rho \epsilon_{a\rho}^2 + \nu_i^2, \tag{21}$$

$$B_i = (E_b - \mu_i)^2 + \sum_\rho \epsilon_{b\rho}^2 + \nu_i^2, \tag{22}$$

$$G_i = -\epsilon_{a\sigma}(E_a + E_b - 2\mu_i), \tag{23}$$

while for the coefficient linear in ϕ_a one has

$$C_i = -2\sum_{\rho\neq\sigma}(E_a + E_{a+\hat{\rho}} - 2\mu_i)\epsilon_{a\rho}\phi_{a+\hat{\rho}}^i + 2\sum_{\rho+\tau\neq 0}\epsilon_{a\rho}\epsilon_{a+\hat{\rho},\tau}\phi_{a+\hat{\rho}+\hat{\tau}}^i, \tag{24}$$

with a similar equation (replacing a by b) for the coefficient D_i.

Defining diagonal matrices $\mathcal{A}_{ij}=A_i\delta_{ij}$, $\mathcal{B}_{ij}=B_i\delta_{ij}$, $\mathcal{G}_{ij}=G_i\delta_{ij}$, and a $2N_B\times 2N_B$ matrix M by

$$M = \begin{pmatrix} \mathcal{A} & \mathcal{G} \\ \mathcal{G} & \mathcal{B} \end{pmatrix}$$

and a $2N_B$-dimensional column vector containing the coefficients C_i, D_i

$$V = \begin{pmatrix} C \\ D \end{pmatrix},$$

with a similar representation for the fields ϕ_a, ϕ_b:

$$\Phi = \begin{pmatrix} \phi_a \\ \phi_b \end{pmatrix}.$$

The Boltzmann weight for the fields ϕ_a, ϕ_b may be written

$$e^{-\Phi M\Phi - V\Phi} = e^{-(\Phi + VM^{-1}/2)M(\Phi + M^{-1}V/2) + VM^{-1}V/4} \tag{25}$$

$$= e^{-\Psi M\Psi} e^{VM^{-1}V/4} \tag{26}$$

with

$$\Psi \equiv \Phi + \frac{1}{2}M^{-1}V. \tag{27}$$

As the multiboson fields for different index i do not interact, the $2N_B\times 2N_B$ matrix algebra implicit in the above equations actually decouples into N_B independent 2×2 problems. In particular, the total weight for the ϕ_a, ϕ_b field pair, with a particle at either a or b, is found by integrating out these fields:

$$W_{ab} \equiv \int d\Phi\, e^{-\Phi M\Phi - V\Phi} \tag{28}$$

$$= \det{}^{-1/2}(M) e^{VM^{-1}V/4} \tag{29}$$

$$= \prod_i (A_iB_i - G_i^2)^{-1/2} e^{(1/4)(B_iC_i^2 + A_iD_i^2 - 2G_iC_iD_i)/(A_iB_i - G_i^2)}. \tag{30}$$

With these preliminaries, we can now state the procedure needed to implement a coupled heat-bath particle move–multiboson field update. The first step is to determine a relative Boltzmann weight for placing a particle at either site a or site b. This weight is determined as a product of three factors.

(1) If the particle is charged, there is a contribution from the electric field term $\exp[-(\beta/2)\Sigma'_{n\mu}D_{n\mu}^2/\epsilon_{n\mu}]$, where the prime indicates that only lattice links connected to site *a or* site b are included. Here the dependence on particle location is entirely through the change a particle move induces in the dielectric field.

(2) There is a contribution from the dielectric factor $\exp[-(1/2)\Sigma'_{n\mu}\ln(\epsilon_{n\mu})]$, with the same interpretation of the primed sum.

(3) Finally there is a contribution from the multiboson energy $W_{ab}e^{-S_{\text{non-}ab}}$ arising from the total integrated weight W_{ab} of the ϕ_a, ϕ_b fields computed in Eq. (28), together with the portion of the multiboson energy depending on the neighboring multiboson fields ϕ' (which also depend on particle location only through the dielectric field).

A decision on a final location for the particle (either site a or site b) is now made on the basis of the relative weight determined from the product of the three factors described above. Once a particle location has been decided, a new set of multiboson fields on sites a and b are calculated by a heat-bath algorithm by determining Ψ according to the Gaussian Boltzmann weight $e^{-\Psi M \Psi}$, and then setting

$$\Phi = \begin{pmatrix} \phi_a \\ \phi_b \end{pmatrix} = \Psi - \frac{1}{2} M^{-1} V.$$

IV. SIMULATION RESULTS FOR THE COUPLED HEAT-BATH METHOD

We tested the efficiency of our improved simulation technique by simulating a system of 1000 neutral particles on a $16 \times 16 \times 16$ lattice as studied in Ref. [7]. For the simulations of this paper we have chosen the dielectric constant ratio between the particles and the background medium to be 0.05 (in typical molecular dynamics biophysical simulations, for example, the protein interior is given an effective dielectric constant of ≈ 4 while the aqueous medium is ≈ 80). In particular, in the simulations the particles have a dielectric constant of 0.05 and the background dielectric constant is 1.0. The dimensionless inverse temperature is 0.25, as in the previous simulations of this system.

The relevant physical quantity for systems of this type is the structure function defined as the Fourier transform $S(\vec{q})$ of the coordinate space density-density correlation function (Ref. [7]). As we work on a spatial lattice, the allowed momentum magnitude values $q \equiv |\vec{q}|$ are discrete: we have chosen to average the structure factor $S(q)$ over degenerate values of the magnitude of the Fourier momentum vector (on a $16 \times 16 \times 16$ lattice, there are 115 nonzero distinct allowed values). This data set is measured every ten sweeps, and error bars extracted at the end of the runs by blocking the measurements in order to take autocorrelations into effect. This allows a measurement of a χ^2 goodness of fit of the final averaged data to the exact answer, which for neutral dielectric particles is simply a flat structure function

$$S(q) = N\left(1 - \frac{N-1}{V-1}\right), \quad q \neq 0,$$

where N is the number of particles and V the number of spatial points on the lattice.

As emphasized in Sec. II, the choice of the number N_B of multiboson fields introduced to model the dielectric contribution to the partition function is dictated by the need to properly describe the low (infrared) part of the spectrum of the Poisson operator $\mathcal{M}$, which contains eigenvalues of order $1/L^2$ on $L \times L \times L$ lattices. Too small a choice for N_B can be expected to lead to systematic deviations in the structure factor of Eq. (31) for small momenta q. On the other hand, too large a choice leads to rapidly falling acceptance rates for multiboson updates and is clearly more computationally costly per Monte Carlo update step. The systematic deviation in the structure factor resulting from too small a choice for N_B is shown in Fig. 1, where we compare the structure factors on a $16 \times 16 \times 16$ lattice for $N_B = 4, 8, 16$. It is clear that for this problem, four multiboson fields are inadequate, giving a distinct curvature to the structure factor, and a large χ^2 per degree of freedom of 36.4, whereas the χ^2 per degree of freedom for the simulation with 16 multiboson fields is only 1.94.

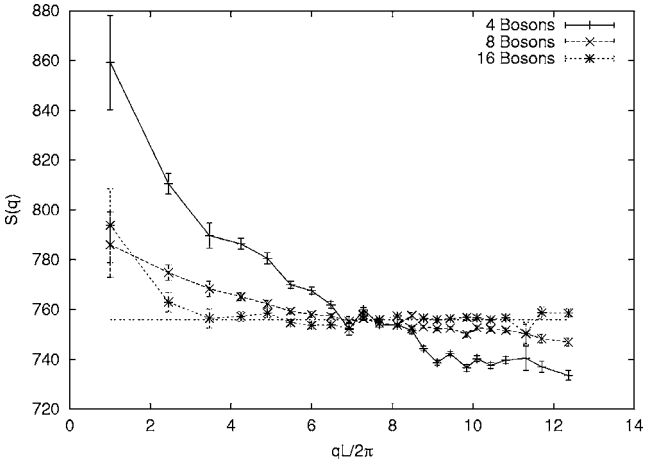

FIG. 1. Structure factor for neutral system calculated using the coupled algorithm. Results are shown for 4, 8, and 16 bosons. 160,000, 400,000, and 800,000 measurement sweeps were used for the runs with 4, 8, and 16 bosons, respectively. For clarity, only every fifth wave number q is plotted.

Depending on the physical parameter regime, and the size of lattice used, it will evidently be necessary to increase N_B to achieve adequate accuracy, at least for long-range features of the physics. Unfortunately, the update procedure introduced in Ref. [7] suffers from the drawback that, for fixed physical parameters (lattice size, dielectric constant, etc.), the acceptance rates for multiboson updates decreases exponentially rapidly with N_B. This makes the uncoupled multiboson method impractical for much larger lattices than those studied in our previous work. In Fig. 2 we compare the acceptance rates using the original update procedure, in which

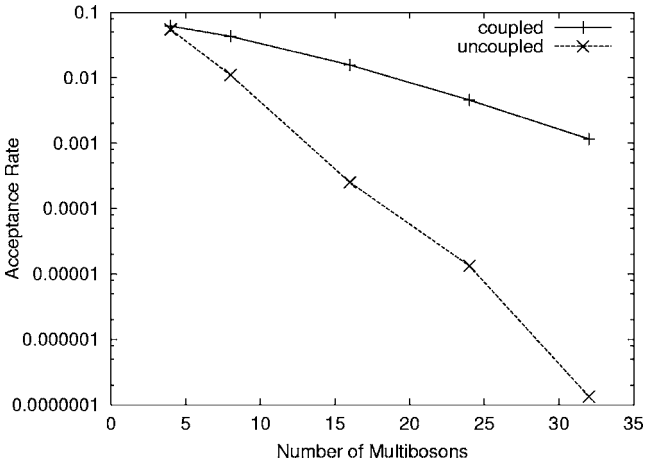

FIG. 2. Acceptance rates for particle moves as a function of number of multibosons, shown for both earlier algorithm where the multiboson updates and particle updates are uncoupled and the improved coupled algorithm.

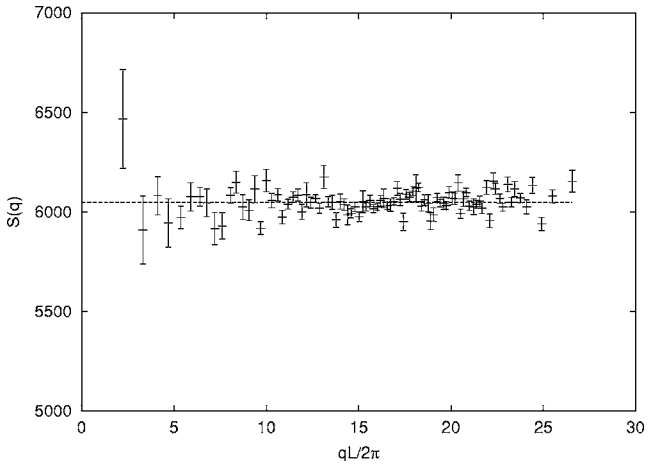

FIG. 3. Structure factor for neutral system calculated using the coupled algorithm with 16 bosons on a $32\times32\times32$ lattice. 40,000 measurement sweeps were used.

particle moves were decoupled from updates of the multiboson fields, with the acceptance rates using the procedure described in Sec. III, in which particle moves are coupled to readjustments in the multiboson field. For larger values of N_B it is clear that the acceptance rates are increased by orders of magnitude (e.g., by about 10^4 for $N_B=32$).

To demonstrate the applicability of our methods on larger systems, we show in Fig. 3 the structure factor calculated from a short run on a larger $32\times32\times32$ lattice with $N_B=16$ (this lattice is similar in size to those used in recent simulations of ion channel properties [10]). The system has 8000 particles so that the particle density remains the same as on our $16\times16\times16$ lattice. With only a modest increase in the number of multiboson fields we are able to obtain a flat structure function on this larger lattice. This simulation, as well as the others discussed in this paper, was conducted on a workstation. Significantly larger systems could be studied using a supercomputer or cluster of workstations as the algorithm discussed here is local, and therefore easily parallelized.

Although the coupled procedure is more computationally intensive, it does not require significantly more computational time per Monte Carlo sweep. We observe that for a run with the parameters described above with 16 bosons, the computational time per Monte Carlo sweep using the coupled update method is only about 13% greater than in the original uncoupled algorithm. This additional computational cost is insignificant given the great increase in particle move acceptances that the coupled method provides. As for correlation times, we note that the heat-bath update procedure used for the electric and multiboson fields is the same as in the original algorithm of Ref. [7]: these fields decorrelate rapidly (on the order of a few sweeps). The increase in particle acceptance rates in the accelerated algorithm described here results in lower correlation times for observables involving the particle locations. For the structure factor, the improvement in correlation time depends on the momentum. For the $\vec{q}=(0,0,1)$ component (on the $16\times16\times16$ lattice) the correlation time is reduced from approximately 15000 sweeps in the original algorithm to 1800 sweeps in the accelerated, coupled algorithm, almost a factor of 10. For higher-momentum components such as $\vec{q}=(0,0,5)$ the reduction is even greater, a factor of 200.

V. CONCLUSION

By using an update method where the proposed particle moves include a relaxation of the multiboson field to adjust to the change in particle location we have been able to dramatically increase the acceptance rates for larger systems that require a larger number N_B of multiboson fields to accurately model the long-wavelength physics of the system. For both the original uncoupled and the improved coupled update algorithms, and for the physical parameters used here, the dependence of the acceptance rate on N_B is exponential $[\exp(-KN_B)]$. The coefficient in the exponent K is $\simeq0.13$ for the coupled algorithm and $\simeq0.46$ for the original method, amounting to a difference in acceptance rates of four orders of magnitude for a simulation with 32 multiboson fields. Tests done with charged particles show similar improvements to the acceptance rates, although for some parameter regions the electric field must also be coupled into the particle moves to obtain reasonable acceptance rates [6].

ACKNOWLEDGMENTS

The work of A. Duncan was supported in part by NSF Grant No. PHY0244599. The work of R. D. Sedgewick was supported in part by the David and Lucile Packard Foundation.

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