Local simulation algorithms for Coulomb gases with dynamical dielectric effects

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We discuss the application of the local lattice technique of Maggs and Rossetto [Phys. Rev. Lett. **88**, 196402 (2002)] to problems that involve the motion of objects with different dielectric constants than the background. In these systems, the simulation method produces a spurious interaction force which causes the particles to move in an unphysical manner. We show that this term can be removed using a variant of a method known from high-energy physics simulations, the multiboson method, and demonstrate the effectiveness of this corrective method on a system of neutral particles. We then apply our method to a one-component plasma to show the effect of the spurious interaction term on a charged system.

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I. INTRODUCTION

The long-range character of the electrostatic Coulomb interaction lies at the root of the computational difficulties encountered in the simulation of many systems of biophysical interest, in which one wishes to understand the thermodynamics of a Coulomb gas of charged particles—or macroions—moving in an environment of spatially varying dielectric. Recently, Maggs and collaborators [1–4] have suggested rewriting the problem of a classical Coulomb gas in a local lattice framework in which each charged particle responds only to the local electric field, which is also updated so that Gauss's law is respected at each point in the simulation. Most applications of the original local algorithm, as well as a variety of suggested improvements [5,6], have dealt primarily with situations in which the dielectric constant is not spatially varying. In this case, the transverse (or "curl") part of the electric field, which is unconstrained in the partition sum, decouples from the physics of the charged ions, so that the method correctly calculates the classical electrostatic energy of the charges.

In this paper, we consider situations in which the dielectric constant becomes dynamical: i.e., is spatially varying, and in a way that depends on the location of the charges in the system, so that it changes in the course of the Monte Carlo simulation. In a molecular dynamics simulation, for example, one effectively determines the electrostatic energy of the system at each step by solving the appropriate Poisson equation (in the presence of the varying dielectric). Of course, the resulting energy expression still suffers from the problem of having to include contributions from all pairs of charged particles in the system. In the local lattice approach, on the other hand, the unconstrained transverse part of the functional integral over the electric field no longer decouples from the charged particle dynamics and leads [2] to an apparent attractive dipole-dipole interaction, even when the system is completely electrically neutral, with zero classical electrostatic energy. Although such interactions certainly exist at a quantum level (e.g., Casimir, Keesom, van der Waals forces), our interest here is in a purely classical calculation.

Our purpose in this paper is to show that the local algorithm of Maggs *et al.* can be extended by addition of a set of boson fields—with a completely local Hamiltonian—which remove any unphysical contributions from the curl part of the electric field, so that the thermodynamics reflects the classical partition function of a charged system with electrostatic energy $H_{\rm es}=\int d\vec{r}(\vec{D}^2/2\epsilon(\vec{r}))$, as desired. In Sec. II, we describe in detail the structure of the transverse field contribution in a local lattice formulation of the Coulomb gas. In particular, we derive the form of the determinant induced by this contribution. In Sec. III, we describe the use of a multiboson technique familiar in lattice gauge theory ("unquenched" quantum chromodynamics) to eliminate the spurious determinant factor. In Sec. IV, we test the method by calculating the density-density structure factor, both with a system of neutral dielectric particles and with a one-component charged plasma. Finally, in Sec. V, we summarize our results and discuss the outlook for further applications.

II. TRANSVERSE MODE CONTRIBUTIONS IN SYSTEMS WITH VARYING DIELECTRIC

In this section, we shall show how the local algorithm of references [1–6] can be modified to prevent the appearance of spurious dipolelike interactions that are not present in the classical electrostatics of the system when the dielectric constant varies both spatially and in the course of the simulation (e.g., if there are mobile entities with dielectric different from that of the ambient medium). We illustrate the point first in the case of a continuous system. Later, a spatial lattice will be introduced to make the functional integrations precise.

Consider the partition function of a system consisting of N free charges (mobile or fixed) e_i at locations $\vec{r}_i$, thereby producing 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) $\epsilon(\vec{r})$. Note that in general the dielectric function $\epsilon(\vec{r})$ may depend on the locations of the free charges $\vec{r}_i$, which may be embedded in regions of vary-

ing dielectric. This dependence should be kept in mind, although for notational convenience it will be suppressed in the following. The electric displacement can be broken 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, we have

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

If the constraint of Maxwell's second law is explicitly imposed the transverse part of the electric displacement vanishes and the electrostatic energy of the system is given by

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

and 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.

On the other hand, the partition function proposed in Ref. [2] includes an integral over both the transverse and longitudinal parts of the electric displacement and reads simply

$$Z' = \int \prod_{i=1}^{N} d\vec{r}_i \prod_{\vec{r}} \mathcal{D}\vec{D}(\vec{r})\,\delta(\vec{\nabla}\cdot\vec{D} - \rho(\vec{r}))e^{-(\beta/2)\int d\vec{r}\vec{D}^2/\epsilon(\vec{r})} \tag{7}$$

$$= \int \prod_{i=1}^{N} d\vec{r}_i \prod_{\vec{r}} \mathcal{D}\vec{D}^{\parallel}(\vec{r})\mathcal{D}\vec{D}^{\mathrm{tr}}(\vec{r})\,\delta(\vec{\nabla}\cdot\vec{D}^{\parallel} - \rho(\vec{r})) \times e^{-(\beta/2)\int d\vec{r}\vec{D}^{\parallel}(\vec{r})^2/\epsilon(\vec{r})} e^{-(\beta/2)\int d\vec{r}\vec{D}^{\mathrm{tr}}(\vec{r})^2/\epsilon(\vec{r})} \tag{8}$$

as a result of the identity Eq. (4). It is apparent that the integration over transverse degrees of freedom $\vec{D}^{\mathrm{tr}}$ in Eq. (8) necessarily introduces a dependence on the particle locations $\vec{r}_i$ through the dependence on $\epsilon(\vec{r})$ absent in the conventional electrostatic energy of Eq. (5). The exact form of this spurious ϵ dependence can be uncovered by considering the form of Z' for the special case $e_i=0$ of uncharged particles, where $D^{\parallel}=0$ and the entire dependence on $\epsilon(\vec{r})$ derives from the transverse part of the functional integral in Z'.

Of course, in the real world quantum fluctuations of the transverse (and longitudinal) parts of the field do exist, and would have to be included in a fully quantum-mechanical treatment of the Coulomb gas problem. This is not, however, the problem being addressed here, where we are computing the *purely classical* partition function of a classical Coulomb gas. Accordingly, the spurious interaction potentials induced by the integration over transverse degrees of freedom in Eq. (8) should not be identified with Keesom potentials, for example, which have a quantum mechanical origin, and a strength dependent on Planck's constant, which appears nowhere in our classical partition function. Such non-Coulombic potentials (whatever their origin—classical or quantum) can, of course, be included phenomenologically in our classical treatment as an explicit separate contribution to the energy function (with an appropriate phenomenological interaction strength). For example, hydrophobic interactions, which depend on intermolecular forces and thus are quantum mechanical in origin, play a significant role in the organization and function of molecular level biophysical structures (e.g., membranes, proteins, and nucleic acids). Hydrophobic effects can be included empirically by adding to the electrostatic free energy a term proportional (with constant of proportionality often called the "surface tension") to the surface area of the membrane, protein, or nucleic acid that is exposed to water [7,8].

Before investigating the special case of neutral particles, we shall go over to a lattice discretization of the system. We imagine a lattice Coulomb gas with 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. Likewise, it turns out to be convenient to associate a dielectric value with each *link* (rather than site), so that the dielectric function on the lattice becomes $\epsilon_{n\mu}$. For example, in problems involving macroions extending over several lattice sites and with dielectric constant differing from that of the ambient medium, links crossing the surface of the macroion can be chosen to have an appropriately interpolated value of the dielectric constant. Alternatively, this can be regarded as a generalization to allow nonisotropic systems where the principal axes of the dielectric tensor coincide with the lattice axes. The entire discussion given below can readily be generalized to the case of a completely general dielectric tensor field. Introducing left (respectively, right) lattice derivatives $\bar{\Delta}$ (respectively, Δ), the Helmholtz decomposition of the displacement field on the lattice becomes

$$D_{n\mu} = -\epsilon_{n\mu}\Delta_\mu\phi_n + \sum_{\nu\sigma}\epsilon_{\mu\nu\sigma}\bar{\Delta}_\nu A_{n\sigma}, \tag{9}$$

where the electrostatic potential (lattice site field) ϕ_n satisfies the Poisson equation

$$-\sum_{\mu}\bar{\Delta}_\mu(\epsilon_{n\mu}\Delta_\mu\phi_n) = \rho_n, \tag{10}$$

$$\rho_n = \sum_i e_i\delta_{n r_i}. \tag{11}$$

In the absence of free charges, $e_i=0$, the local form of the partition function Z' becomes

$$Z'(e_i=0) \equiv \int \prod_{i=1}^{N} d\vec{r}_i \mathcal{F}(\epsilon), \tag{12}$$

where the ϵ dependence is entirely due to the transverse degrees of freedom and enters through the function

$$\mathcal{F}(\epsilon) = \int \prod_{n\mu} dD_{n\mu} \delta\left(\sum_{\mu} \bar{\Delta}_\mu D_{n\mu}\right) e^{-(\beta/2)\Sigma_{n\mu} D_{n\mu}^2/\epsilon_{n\mu}} \tag{13}$$

$$= \int \prod_{n} d\lambda_n \prod_{n\mu} dD_{n\mu} e^{i\Sigma_n \lambda_n \bar{\Delta}_\mu D_{n\mu} - (\beta/2)\Sigma_n D_{n\mu}^2/\epsilon_{n\mu}} \tag{14}$$

$$= \int \prod_{n} d\lambda_n \prod_{n\mu} dD_{n\mu} e^{-i\Sigma_{n\mu} D_{n\mu}\Delta_\mu \lambda_n - (\beta/2)\Sigma_{n\mu} D_{n\mu}^2/\epsilon_{n\mu}} \tag{15}$$

$$= C \prod_{n\mu} \sqrt{\epsilon_{n\mu}} \int \prod_{n} d\lambda_n e^{-(1/2\beta)\Sigma_{n\mu}\epsilon_{n\mu}(\Delta_\mu \lambda_n)^2} \tag{16}$$

$$= C' \prod_{n\mu} \sqrt{\epsilon_{n\mu}} \det{}^{-1/2}\left(-\sum_{\mu} \bar{\Delta}_\mu \epsilon_\mu \Delta_\mu\right). \tag{17}$$

In going from (13) and (14), we have introduced an auxiliary field λ_n to implement the Gauss's law constraint (for an everywhere neutral system), allowing the Gaussian integration over the displacement field $D_{n\mu}$ to be carried out explicitly. The constants C and C' are independent of ϵ and of no further interest. The integration over the auxiliary λ_n field (also Gaussian) then yields the determinant of the indicated operator, whose action on a lattice site field takes the explicit form

$$\mathcal{M}\lambda_n \equiv \left(-\sum_{\mu} \bar{\Delta}_\mu \epsilon_\mu \Delta_\mu\right)\lambda_n = \sum_{i=1}^{6} \epsilon_{ni}\lambda_n - \sum_{i=1}^{6} \epsilon_{ni}\lambda_{n+i}, \tag{18}$$

where the index i now runs over both positive ($i=1,2,3$) and negative ($i=4,5,6$) spatial directions, and $\epsilon_{ni} \equiv \epsilon_{n+i,i-3}$ for $i=4,5,6$.

In order to generate an ensemble of configurations based on the partition function Eq. (6) arising from the purely physical electrostatic energy, the spurious functional dependence of $\mathcal{F}(\epsilon)$ must be removed: in other words, we should insert a factor

$$\mathcal{F}^{-1}(\epsilon) = e^{-(1/2)\Sigma_{n\mu} \log(\epsilon_{n\mu})} \det{}^{+1/2}(\mathcal{M}) \tag{19}$$

into the partition integral (7) to remove the effect of the transverse field modes. In the event that the dielectric function is truly spatially independent, or is spatially varying but frozen throughout the simulation, adding the factor of $\mathcal{F}^{-1}(\epsilon)$ is unnecessary, as the transverse integration decouples from the dynamics of the problem.

The problem that we are faced with here is well known: positive (fractional or integral) powers of determinants of local operators are intrinsically nonlocal, unlike negative powers, which may be reexpressed as integrals over auxiliary fields with local actions [cf. Eqs. (13) through (17)]. In lattice quantum chromodynamics (QCD), for example, the inclusion of virtual quark-antiquark processes leads to precisely the positive power of the determinant of the Dirac operator in the path integral for the system, greatly increasing the difficulty of simulations in the full ("unquenched") version of the theory in comparison to the truncated ("quenched") version where the quark determinant is simply dropped [10].

In the next section, we shall show how the multiboson technique introduced by Lüscher [9] for approximately computing the positive power of quark determinants can be used to write a *purely local* Hamiltonian in terms of a set of auxiliary scalars ("multibosons" in the lattice QCD language) which is readily susceptible to Monte Carlo simulation and will allow us to implement the correct electrostatic partition function (6) for systems with general dielectric makeup.

III. ELIMINATION OF TRANSVERSE CONTRIBUTIONS USING MULTIBOSON FIELDS

The representation of determinants of local operators by integrals over multiple auxiliary scalar fields was first introduced by Lüscher *et al.*[9] in the context of unquenched lattice QCD. The essential point is to find a uniform polynominal approximation to the function $1/s$ in the interval $[\delta,1]$ for small δ. In terms of the complex roots of the polynominal $z_k=\mu_k+i\nu_k$, a convenient choice is the Chebyshev polynominal of order $2N_B$ with

$$\frac{1}{s} \simeq P(s) \equiv C\prod_{k=1}^{N_B}\left[(s-\mu_k)^2+\nu_k^2\right], \tag{20}$$

$$\mu_k = \frac{1}{2}(1+\delta)\left(1-\cos\frac{2\pi k}{2N_B+1}\right), \tag{21}$$

$$\nu_k = \sqrt{\delta}\sin\frac{2\pi k}{2N_B+1}. \tag{22}$$

The representation of Eq. (20) can be extended to the determinant of a real positive symmetric operator with spectrum in the interval [0,1]

$$\det{}^{+1/2}(\mathcal{M}) \simeq \prod_{k=1}^{N_B} \det{}^{-1/2}\left[(\mathcal{M}-\mu_k)^2+\nu_k^2\right], \tag{23}$$

where the representation becomes exact in the limit $N_B\to\infty, \delta\to 0$. However, we shall see that accurate results can be obtained with surprisingly small values of N_B (=number of auxiliary scalar fields, see below).

The essential idea of the multiboson approach is to replace the determinant factors on the right of Eq. (23) by integrals over a set of auxiliary fields $\phi_n^{(k)}$, $k=1,2,\ldots,N_B$, with *local actions*, as follows

$$\prod_{k=1}^{N_B} \det{}^{-1/2}\left[(\mathcal{M}-\mu_k)^2+\nu_k^2\right] = C\int \prod_{k=1}^{N_B} \mathcal{D}\phi^{(k)} e^{-\Sigma_{k=1}^{N_B}\phi^{(k)}((\mathcal{M}-\mu_k)^2+\nu_k^2)\phi^{(k)}}, \quad (24)$$

where, once again, C is an irrelevant constant that can henceforth be neglected. As pointed out previously, our polynominal representation assumes that the spectrum of the operator $\mathcal{M}$ in Eq. (24) lies in the interval [0,1]. Let us assume that the dielectric function ϵ of our system is bounded above by the value ϵ_0 (frequently, in biophysical simulations, this is $\simeq$80, corresponding to the dielectric constant of an aqueous ambient medium). Recalling that the lattice Laplacian operator has largest eigenvalue equal to 12, one easily shows that the operator

$$\mathcal{M} \equiv \frac{1}{K\epsilon_0}(-\bar{\Delta}_\mu \epsilon_\mu \Delta_\mu) \quad (25)$$

has a spectrum contained in the unit interval provided $K \geqslant 12$. In the multiboson approach, the auxiliary scalar field $\phi^{(k)}$ is entrusted with resolving the spectrum of the operator $\mathcal{M}$ in the neighborhood of μ_k in a region of width ν_k (see Ref. [9]). For k near 1 or N_B, ν_k is small and μ_k is close to zero or one, and only a small region of the spectrum is accurately treated. We can eliminate the lack of resolution for finite N_B at the upper end of the spectrum by choosing K somewhat larger than 12 (in the simulations reported below, we typically take $K=13$), but if the spectrum of $\mathcal{M}$ is very dense near the origin, we will necessarily be forced to use a large value of N_B. Fortunately, in the systems we have so far simulated, this does not appear to be the case. This is a fortunate distinction from the case of lattice quantum chromodynamics, where chiral symmetry breaking necessarily implies a dense spectrum of eigenvalues of the quark Dirac operator at the origin. Instead, in the systems of concern to us, the region with large dielectric ϵ_0 occupies almost all of the volume of the system, and the spectral density of $\mathcal{M}$ does not differ appreciably from that of the free Laplacian.

To summarize our proposal, we shall consider a system of mobile charged entities (charges e_i, locations $\vec{r}_i$) with total Hamiltonian

$$H_{\mathrm{tot}} = H_{\mathrm{es}} + V_{\mathrm{nc}}(\vec{r}_i), \quad (26)$$

where the purely electrostatic energy H_{es} is given in Eq. (5), while all other non-Coulombic energy effects (exclusion, Keesom, van der Waals, hard core, soft core, etc.) are included in V_{nc}, with appropriate phenomenological values. The latter are not typically problematic as they are essentially short-range effects. From Eqs. (17), (19), and (24), we find that the correct expression for the partition function is

$$Z = \int \prod_i d\vec{r}_i \prod_{n\mu} dD_{n\mu}\, \delta\left(\sum_\mu \bar{\Delta}_\mu D_{n\mu} - \rho_n\right) \times \mathcal{F}^{-1}(\epsilon) e^{-\beta V_{\mathrm{nc}}} e^{-(\beta/2)\Sigma_{n\mu} D_{n\mu}^2/\epsilon_{n\mu}}, \quad (27)$$

$$= \int \prod_i d\vec{r}_i \prod_{n\mu} dD_{n\mu} \prod_{kn} d\phi_n^{(k)}\, \delta\left(\sum_\mu \bar{\Delta}_\mu D_{n\mu} - \rho_n\right) \times e^{-\beta V_{\mathrm{nc}} - (1/2)\Sigma_{n\mu}\log(\epsilon_{n\mu})} e^{-(\beta/2)\Sigma_{n\mu} D_{n\mu}^2/\epsilon_{n\mu}} \times e^{-\Sigma_{k=1}^{N_B}\phi^{(k)}((\mathcal{M}-\mu_k)^2+\nu_k^2)\phi^{(k)}}, \quad (28)$$

where $\mathcal{M}$ is scaled as in Eq. (25) and the integrals over $\vec{r}_i$ are taken to be sums when the charges are constrained to be on lattice sites. The effective Hamiltonian appearing in the exponent terms of (28) is completely local: to simulate the system, we need only update, in some conveniently chosen order, (i) the locations $\vec{r}_i$ of the charged entities, (ii) the lattice displacement field $D_{n\mu}$ (respecting locally the Gauss's law constraint), and (iii) the N_B auxiliary scalar fields $\phi^{(k)}$, in all cases according to the indicated Boltzmann weight.

IV. RESULTS

In order to see the effect of the additional dipolelike interaction present in the uncorrected simulation and study the effectiveness of our correction scheme, we have simulated a system of neutral particles similar to the system studied in Ref. [2]. In classical electrodynamics, neutral particles, even those with a different dielectric constant from the background, do not interact and, therefore, the density-density structure factor, $S(q)$, is constant as a function of q. In contrast, the simulations in Ref. [2] show that using the local lattice approach (not corrected to remove the extra dipole term) to simulate neutral particles with different dielectric constants from the background results in a clearly nonconstant density-density structure factor. In this section, we show that the multiboson method presented in this paper is able to effectively remove the dipole terms so that the neutral particle simulation gives a constant density-density structure factor. We then apply the method to the more interesting case of a one-component plasma with charged particles of different dielectric constant than the background.

In the simulations described below, we have compared the effect of using varying number of multiboson fields to determine the sensitivity of our results to the low eigenvalues of the operator $\mathcal{M}$ discussed in the preceding section. In particular, we have simulated neutral systems with $N_B=4$ boson fields (and $\delta=0.07$) and charged systems with $N_B=4$, 6, 8 (and $\delta=0.07$, 0.07, and 0.05, respectively). It is instructive to see the accuracy of the polynominal approximation $P(s)$ to $1/s$ for these choices by plotting the residual $P(s)-1/s$, as shown in Fig. 1.

We first consider a system of 1000 neutral particles on a 16^3 lattice. The particles are constrained to the lattice site and only one particle is allowed on each lattice site. The background dielectric constant was set to 1.0, and the dielectric constant of the particles was set to 0.2, except in the uniform dielectric simulations where the particles had dielectric constant 1.0. The dielectric constant along a link in the μ direction from a lattice site n is defined through the relation

$$\frac{2}{\epsilon_{n\mu}} = \frac{1}{\epsilon_n} + \frac{1}{\epsilon_{n+\mu}}, \quad (29)$$

where ϵ_n and $\epsilon_{n+\mu}$ are either the background dielectric constant or the particle dielectric constant depending on whether

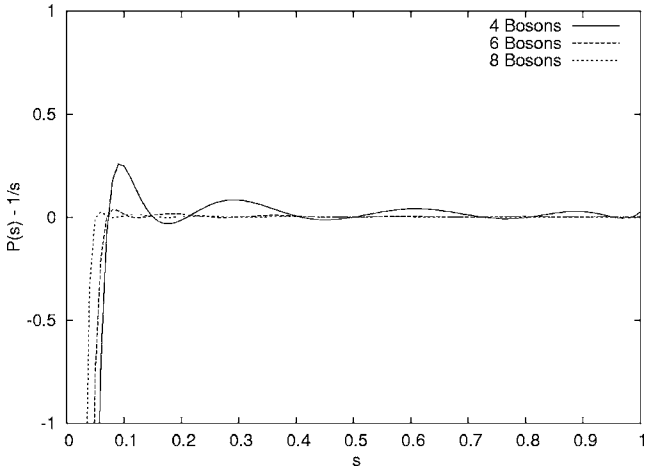

FIG. 1. Residual from polynominal approximation used in the multiboson correction factor for the simulations in this paper.

there is a particle on site n or site $n+\mu$, respectively. The dimensionless inverse temperature, $\hat{\beta}=4\pi e^2\beta/a$, was set to 0.25. We performed 5000 Monte Carlo warmup sweeps, followed by 40 000 Monte Carlo sweeps. To update the electric field, we used the local heat bath method discussed in Ref. [5]. To update the neutral particles at each Monte Carlo step we, chose 1000 particles, which we attempt to move using the methods discussed in Sec. III.

Figure 2 shows the density-density structure factor for both the corrected and uncorrected simulation. In the uniform case, the structure factor is independent of q and is given by $N[1-(N-1)/(V-1)]$, where N is the number of particles and V is the volume of the system (the number of points in the lattice). The spurious dipolelike interactions present in the uncorrected simulation give a density-density structure factor that differs significantly from the desired flat structure factor of the uniform case, while the simulation with the multiboson correction reproduces the analytically calculated flat structure factor of the neutral system. The acceptance rate for particle moves drops from 30% in the uncorrected simulation to 15% in the multiboson simulation. The uncorrected simulation took 11 h to run on a single processor workstation and the corrected simulation took 55 h on a similar workstation.

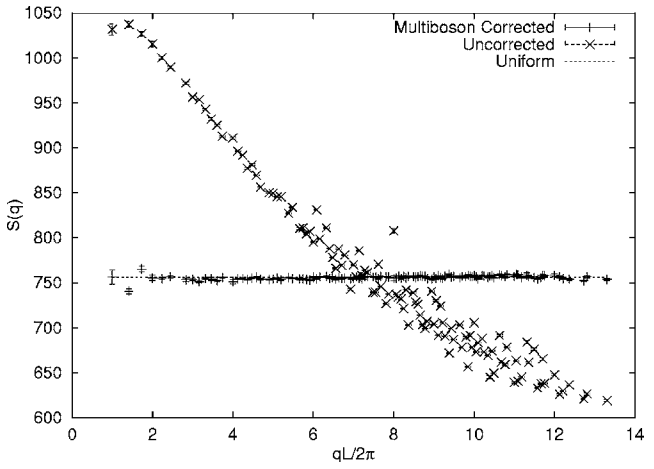

FIG. 2. Density-density structure factor for the neutral system. Shown are the results from both a simulation with the multiboson correction factor and an uncorrected simulation. The dotted line gives the desired q independant structure factor.

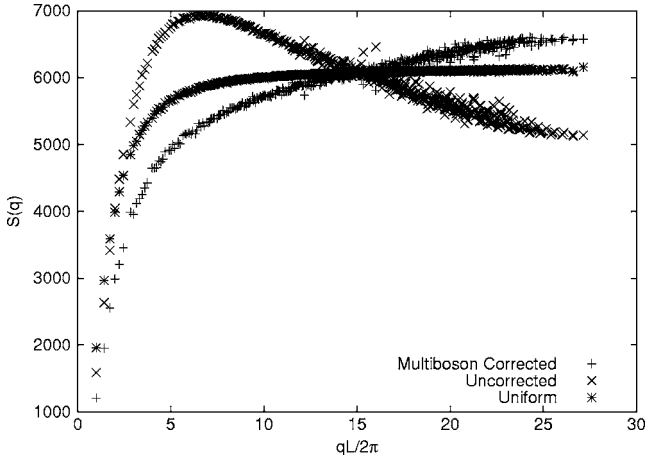

FIG. 3. Density-density structure factor for the charged particles in the one-component plasma. Shown are the results from the uncorrected simulation, the simulation with the multiboson correction factor, and a simulation where the dielectric constant is uniform. The errorbars are smaller than the symbol size.

After verifying that the multiboson method was able to correctly remove the nonphysical dipole interaction from the simulation of neutral particles, we applied the multiboson technique to the simulation of a one-component charged plasma. The particles in the system are positively charged with one electron charge each and the background sites are uniformly given enough negative charge so that the entire system is charge neutral. The parameters of the system are the same as in the neutral particle case except the lattice is a 32^3 lattice, there are 8000 particles are updated each Monte Carlo step, and the dielectric constant of the particles in the nonuniform case was taken to be 0.05. In this case, we have also repeated the simulations with varying numbers of boson fields (N_B=4,6,8).

In Fig. 3, we show the results for the density-density structure function for three cases: the fully multiboson corrected structure function for this system, the uncorrected structure function switching off multiboson contributions, and for a charged plasma with uniform dielectric ($\epsilon_{\text{part}}=\epsilon_{\text{bg}}=1.0$). It is apparent from the figure that the removal of the spurious interactions induced by the transverse part of the field in the nonuniform dielectric case results in a qualitative modification of the shape of the structure function. Also, the results differ significantly between the cases of uniform and nonuniform dielectric. This difference may play an important role in the behavior of systems from biological and chemical physics, so it is important to be able to reliably calculate the effect of having a nonuniform dielectric *which changes dynamically in the course of the simulation*. The results in Fig. 3 were obtained using N_B=4 multiboson fields to estimate the transverse electric field determinant.

Of course, the polynominal approximation Eq. (20) cannot accurately represent very small eigenvalues of $\mathcal{M}$, so it

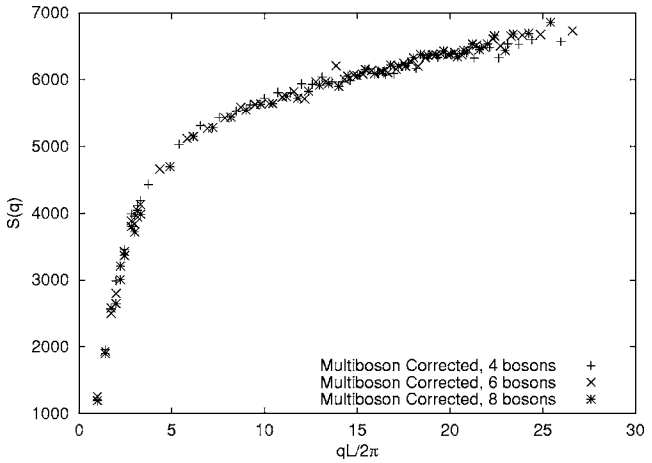

FIG. 4. Density-density structure factor for the charged particles in the one-component plasma. Shown are the results from simulations corrected with differing numbers of bosonic field in the multiboson correc- tion factor. The errorbars are smaller then the symbol size. Only a portion of the larger q results are shown to improve the legibility of the plot.

is important to check the sensitivity of our results to the number of boson fields used. This comparison, again for the case of the charged one-component plasma on a 32^3 lattice described above, is shown in Fig. 4. Certainly the results for N_B=4, 6, and 8 are in complete qualitative agreement over the entire range of q. For larger lattices, one will need to increase N_B to deal with the larger dynamical range in the eigenspectrum of $\mathcal{M}$, and, as we saw previously, this in turn results in a drop in the acceptance rate for particle moves. A similar problem in the use of multiboson fields in unquenched QCD has been addressed [11] by use of a hybrid scheme in which the number of multiboson fields is held fixed, and the low eigenvalues of $\mathcal{M}$ treated exactly by a Lanczos algorithm.

V. CONCLUSION

Systems from biological and chemical physics frequently have mobile charged elements with different dielectric constant from the background. The local lattice approach provides an efficient method to simulate these systems. Unfortunately, a spurious force remains as an artifact of the simulation method. This force can be efficiently removed using a set of bosonic fields to approximate a nonlocal counteracting force. This method is able to effectively remove the spurious term in both neutral and charged systems.

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