Large Fluctuations in Nonideal Coarse-Grained Systems

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Using the recently introduced molecular dynamics lattice gas approach, we test fluctuations of coarse-grained quantities. We show that as soon as the system can no longer be considered an ideal gas fluctuations fail to diminish upon coarse graining as is usually expected. These results suggest that current approaches to simulating fluctuating hydrodynamics may have to be augmented to achieve quantitative results for systems with a nonideal equation of state. The molecular dynamics lattice gas method gives a guidance to the exact nature of the fluctuation in such systems.

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Predicting fluctuations at small scales for coarse-grained systems can be challenging [1–3]. Typically theoretical predictions exist for fluctuations in the hydrodynamic (i.e., long wavelength) limit [4] that can be used to tune fluctuation terms, which is the basis of the Langevin approach to fluctuations [5]. Fluctuating terms in the governing equations are usually assumed to be spatially uncorrelated. The hydrodynamic behavior has to emerge from the local fluctuations introduced into the system. To complicate the situation fluctuations are often most relevant at scales much smaller than the hydrodynamic length scales. This makes it imperative to develop methods that are able to reproduce correct fluctuations at much smaller length scales [2]. It is generally not known what form the small-scale fluctuations for such a coarse-grained system should take. This is a general problem that arises in most simulation contexts where fluctuations are important.

One obvious way to address this shortfall is to use information from a microscopic model, e.g., a molecular dynamics (MD) simulation, to measure the small-scale fluctuations [1]. This information can then be used to tune the fluctuating terms in a coarse-grained simulation method [2]. In this Letter we show that it is possible to go a step further and use a coarse-graining mapping between a MD simulation and a coarse-grained mesoscopic model to directly measure the correct fluctuations of the model variables for different coarse-graining scales. Our results indicate that fluctuations of the model variables can be orders of magnitude larger than was previously expected.

In this Letter we focus on predictions for fluctuating lattice Boltzmann approaches, although we stress that the mapping approach is far more general and can be applied to most other coarse-grained models. For the special case of an ideal gas fluctuations are fairly well understood. This is why this is usually taken as a starting point, e.g., for fluctuating lattice Boltzmann methods [6–9]. For other systems fluctuations arise from the discrete nature of the representation as in lattice gases [4,10] or stochastic rotation dynamics [11,12]. Other discrete versions like dissipative particle dynamics [13–15] include tunable fluctuating forces. For nonideal systems, however, it is typically less clear what the correct fluctuations should look like [16–19]. Because of this difficulty we developed a direct mapping from molecular dynamics onto a lattice gas (MDLG) [20] where fluctuations in a nonideal coarse-grained system can be easily observed. In this Letter we show the results of applying MDLG to analyzing equilibrium fluctuations at different densities of a system of Lenard-Jones (LJ) particles.

The direct mapping between MD and a lattice gas leads to an integer lattice gas. Integer lattice gases exist, but are somewhat rare [10,21–25]. Blommel and Wagner showed that an integer lattice gas can closely model the fluctuations of an ideal gas [10]. Such lattice gases have occupation numbers $n_i(x,t)$ as their fundamental variables. They are defined on lattice points x and are associated with lattice velocities v_i such that $x+v_i$ is again a lattice position. The evolution equation of a lattice gas can be written as

$$n_i(x+v_i, t+\Delta t) = n_i(x,t) + \Xi_i, \tag{1}$$

where the Ξ_i is the lattice gas collision operator. We also define the number density $N=\sum_i n_i$. For the integer lattice gas of Blommel and Wagner [10], the n_i follow the expectation for an ideal gas [26] and are Poisson distributed,

$$P(n_i) = \exp(-f_i^{\mathrm{eq}})(f_i^{\mathrm{eq}})^{n_i}/n_i!, \tag{2}$$

where $f_i^{\mathrm{eq}} = \langle n_i \rangle$. The number density N is similarly Poisson distributed with average $N^{\mathrm{eq}} = \sum_i f_i^{\mathrm{eq}}$.

To examine the fluctuation behavior of a nonideal system (as represented by a MD simulation) we employ the MDLG approach. Here a lattice is superimposed on the MD simulation and the displacement of particles from one lattice cell to another a distance v_i away during a time step Δt is then identified with the lattice gas occupation number n_i. This provides us with a lattice gas that exactly represents the underlying MD system [20]. Explicitly, if $x_j(t)$ is the position of the jth particle at time t, we write

$$n_i(x,t) = \sum_{j=1}^{M} \Delta_x[x_j(t)]\Delta_{x-v_i}[x_j(t-\Delta t)], \tag{3}$$

where $\Delta_y[x]$ is one if $x_\alpha \in [y_\alpha, y_\alpha + \Delta x]$ and zero otherwise for all coordinates α, and M is the total number of particles.

We have previously shown [27] that a MDLG has an equilibrium distribution equivalent to the standard lattice Boltzmann equilibrium distributions when the combination of the time step Δt and lattice size Δx gives

$$a^2 = \frac{\langle \delta(\Delta t)^2 \rangle}{d\Delta x^2} \approx 0.18 \approx \frac{1}{6}, \tag{4}$$

where $\delta(\Delta t)$ represents the displacement of a MD particle in the simulation for a time interval of Δt and d is the number of spatial dimensions. For this choice the equilibrium distribution of MDLG recovers the standard D2Q9 equilibrium distribution of lattice Boltzmann methods for small velocities [28]. To ensure comparability of results to fluctuating lattice Boltzmann implementations [6,7,16,17], we restrict ourselves to this value.

We now examine the equilibrium fluctuations of this lattice gas. For a dilute gas we expect the assumptions of ideal gas fluctuations to hold to good approximation. We perform a molecular dynamics simulation with 99856 particles on a $L^2 = 3000^2$ lattice (measured in LJ units) at a temperature of 50, also in LJ units, as in Ref. [20], to prevent phase separation. The effective radius for excluded volume of $r_c \approx 0.75$ [corresponding to $1/2k_BT = V(r_c)$] implies a volume fraction of $\phi = M\pi r_c^2/(L_x L_y) = 4.9 \times 10^{-3}$ (see Supplemental Material for additional details [29]). For this ϕ we find good agreement between the distribution of the lattice gas occupation numbers and the Poisson distribution, as shown in Fig. 1 for two different lattice spacings Δx.

For larger densities the total density will no longer be Poisson distributed, but follow a narrower distribution. We expect the distribution of the lattice gas occupation numbers n_i to similarly deviate from the Poisson distribution. We performed simulations for a denser system of volume fraction of $\phi = 0.49$. The results shown in Fig. 2(a) show

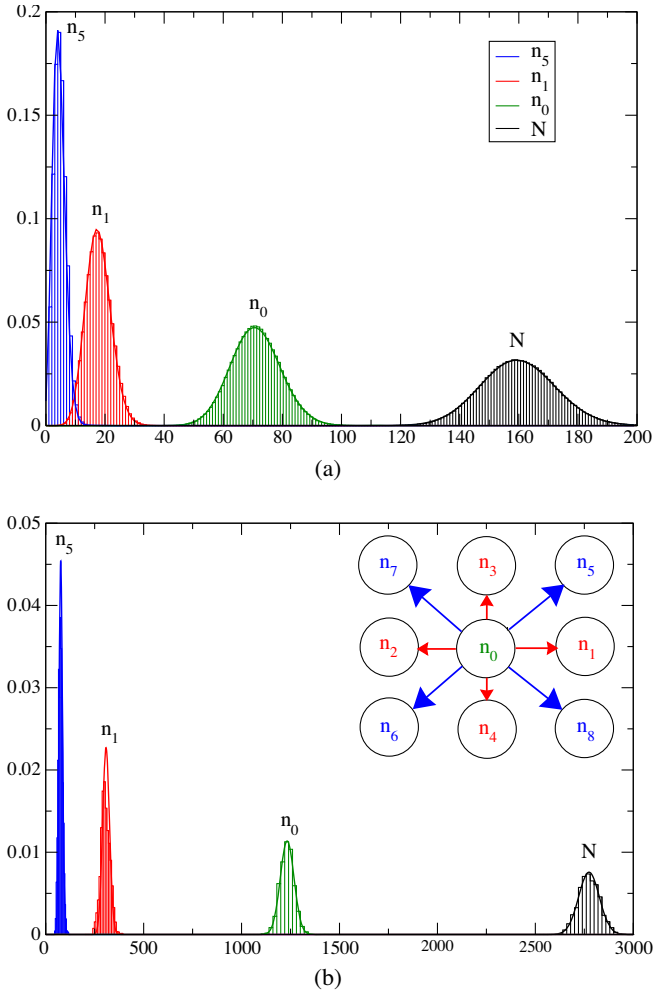

FIG. 1. Distribution of the MDLG occupation numbers n_i and the total density (histograms) compared to the Poisson distribution (solid lines) for volume fraction $\phi \approx 4.9 \times 10^{-3}$ for different lattice spacings (a) $\Delta x = 120$ and (b) $\Delta x = 500$. In (b) we also sketched the numbering of the velocities.

the narrowing of the N distribution, but surprisingly the distribution of rest particles (n_0) appears little changed whereas the distributions of particles moving to nearest neighbors (n_1) as well as diagonal neighbors (n_5) is much wider. We find similar results for three-dimensional simulations, which are reported in the Supplemental Material [29].

For each lattice spacing Δx there is a time step Δt that corresponds to $a^2 = 1/6$. It is therefore essential how the distributions depend on Δx, corresponding to modeling the system at different scales. Increasing Δx will increase the average number of particles per cell N^{eq}. For an ideal system the width of the Poisson distribution will grow only as the square root of N^{eq}, making the distribution more peaked for larger N^{eq}. Therefore, for larger Δx the importance of fluctuations declines. This classical result is found for our the dilute system, as shown in Fig. 1(b).

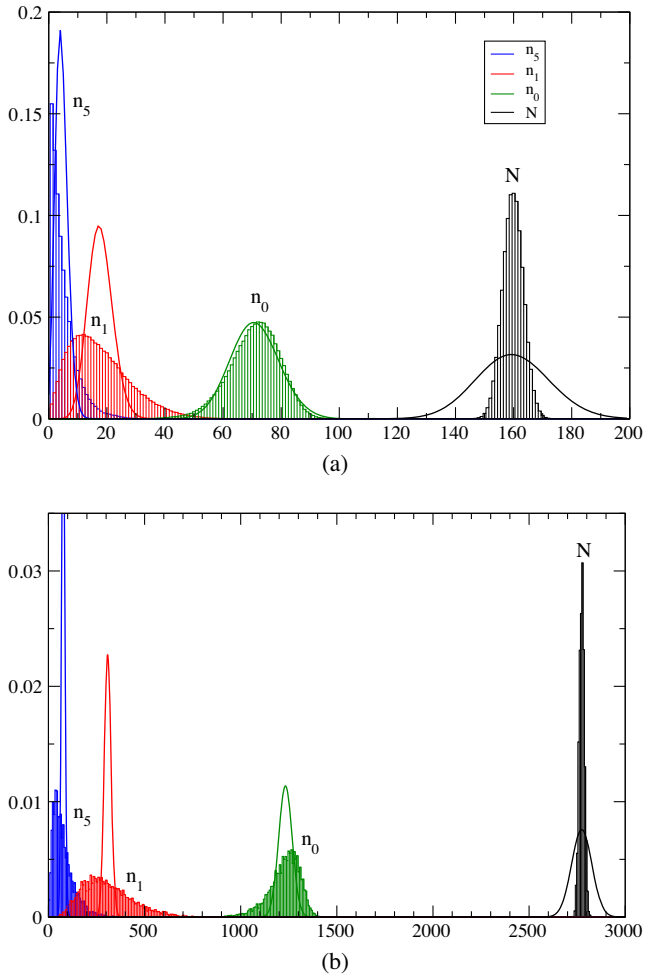

FIG. 2. Distribution of the MDLG occupation numbers n_i and the total density compared to the Poisson distribution for volume fraction $\phi \approx 0.49$ and the lattice spacing is (a) $\Delta x = 12$ and (b) $\Delta x = 50$.

For the dense system of Fig. 2(b) the density does indeed show a sharpening of the normalized width, as one would expect. But the normalized width of the distributions of the n_i barely narrow. This is a counterintuitive result, which suggests that the importance of fluctuations for the n_i does not diminish as $1/\sqrt{M}$ with increasing Δx.

Let us first consider how combining wider distributions for the n_i can lead to a narrower distribution of N. We can write $\langle (N - N^{eq})^2 \rangle = \sum_i \sum_j \langle (n_i - f_i^{eq})(n_j - f_j^{eq}) \rangle$. For an ideal system the distributions of the n_i are independent and $\langle (n_i - f_i^{eq})(n_j - f_j^{eq}) \rangle = f_i^{eq} \delta_{ij}$. But for nonideal systems the wider distributions for the n_i requires that at least for some i and j these correlations must become quite negative to cancel the widening of the distributions for $i = j$.

We express this quantitatively in terms of the probabilities of the particle displacements $\delta_j = x_j(t) - x_j(t - \Delta t)$. We obtain

$$\begin{aligned}\langle n_i \rangle &= \left\langle \sum_{k=1}^{M} \Delta_x[x_k(t)] \Delta_{x-v_i}[x_k(t - \Delta t)] \right\rangle \\ &= M \int dx_1 \int d\delta_1 \cdots \int d\delta_M P^M(x_1, \delta_1, \ldots, x_M, \delta_N) \\ &\quad \times \Delta_x(x_1) \Delta_{x-v_i}(x_1 - \delta_1) \\ &= M \int dx_1 \int d\delta_1 P^1(x_1, \delta_1) \Delta_x(x_1) \Delta_{x-v_i}(x_1 - \delta_1) \\ &= f_i^{eq}, \end{aligned} \tag{5}$$

where we introduced the useful (but not very common) M-particle distribution function for the *displacements* of particles during a time step Δt. We see that the expectation value of the distribution is entirely dependent on the one-particle distribution function. This is the reason that Parsa *et al.* [27] found that the equilibrium distribution depends on the nondimensional mean squared displacement a^2 only.

The probability for finding a specific occupation number n_i is then given by

$$\begin{aligned} P(n_i) &= \int dx_1 \int d\delta_1 \cdots \int d\delta_M P^M(x_1, \delta_1, \ldots, x_M, \delta_M) \\ &\quad \times \Theta(n_i; \{x_1, \delta_1, \ldots, x_M, \delta_M\}) \\ &= \int dx_1 \int d\delta_1 \cdots \int d\delta_M P^M(x_1, \delta_1, \ldots, x_M, \delta_M) \\ &\quad \times \binom{M}{n_i} \Theta(n_i; \{x_1, \delta_1, \ldots, x_{n_1}, \delta_{n_1}\}), \end{aligned} \tag{6}$$

where we define a binary flag that is one if we have the occupation number $n_i(x)$ as

$$\begin{aligned} &\Theta(n_i; \{x_1, \delta_1, \ldots, x_M, \delta_M\}) \\ &\quad = \begin{cases} 1 & \text{if } \sum_{k=1}^{M} \Delta_x(x_k) \Delta_{x-v_i}(x_k - \delta_k) \equiv n_i \\ 0 & \text{else.} \end{cases} \end{aligned} \tag{7}$$

In the special case of an ideal gas, where the M-particle distribution factorizes,

$$P^{M,id}(x_1, \delta_1, \ldots, \delta_M) = \prod_{k=1}^{M} P^1(x_k, \delta_k), \tag{8}$$

we have

$$\begin{aligned} P^{id}(n_i) &= \binom{M}{n_i} \left(\frac{f_i^{eq}}{M} \right)^{n_i} \left(1 - \frac{f_i^{eq}}{M} \right)^{M - n_i} \\ &\approx \exp(-f_i^{eq}) \frac{(f_i^{eq})^{n_i}}{n_i!}, \end{aligned} \tag{9}$$

where the last step is the familiar transition from the binomial distribution to the Poisson distribution in the limit of large M. We can shed light on the expected width of the distribution for the nonideal case by reducing the expression to one for the two-particle distribution function:

$$\begin{aligned}\langle n_i(x)n_j(y)\rangle &= \left\langle \sum_{k=1}^{M} \Delta_x(x_k)\Delta_{x-v_i}(x_k-\delta_k) \sum_{l=1}^{M} \Delta_y(x_l)\Delta_{y-v_j}(x_l-\delta_l) \right\rangle \\ &= \sum_{k,l} \int dx_1 \int d\delta_1 \cdots \int d\delta_M P^M(x_1,\delta_1,\ldots,x_M,\delta_M)\Delta_x(x_k)\Delta_{x-v_i}(x_k-\delta_k)\Delta_y(x_l)\Delta_{y-v_j}(x_l-\delta_l) \\ &= (M^2-M)\int dx_1 \int d\delta_1 \int dx_2 \int d\delta_2 P^2(x_1,\delta_1,x_2,\delta_2)\Delta_x(x_1)\Delta_{x-v_i}(x_1-\delta_1)\Delta_y(x_2)\Delta_{y-v_j}(x_2-\delta_2) \\ &\quad + M\int dx_1 \int d\delta_1 P^1(x_1,\delta_1)\Delta_x(x_1)\Delta_{x-v_i}(x_1-\delta_1)\Delta_y(x_1)\Delta_{y-v_i}(x_1-\delta_1) \\ &= (M^2-M)\int dx_1 \int d\delta_1 \int dx_2 \int d\delta_2 P^2(x_1,\delta_1,x_2,\delta_2)\Delta_x(x_1)\Delta_{x-v_i}(x_1-\delta_1)\Delta_y(x_2)\Delta_{y-v_j}(x_2-\delta_2) \\ &\quad + f_i^{eq}\delta_{ij}\delta_{xy}, \end{aligned} \tag{10}$$

where, for an ideal gas, the two-particle probability factorizes (8). With this, we obtain for an ideal gas

$$\langle n_i(x)n_j(y)\rangle^{\mathrm{id}} = (1-1/M)f_i^{\mathrm{eq}}f_j^{\mathrm{eq}} + f_i^{\mathrm{eq}}\delta_{ij}\delta_{xy}. \tag{11}$$

This is the result that one would expect for an independently binomial distributed n_i. In the limit of a large system with $M \to \infty$ the $1/M$ can be neglected, and we obtain the result predicted for a Poisson distributed n_i.

For dilute gases the representation of the particles as ideal particles works quite well. We define the scaled squared width of the actual distribution as

$$W_{ii} = \langle (n_i(x) - f_i^{\mathrm{eq}})^2\rangle / (N^{\mathrm{eq}} f_i^{\mathrm{eq}}). \tag{12}$$

For a Poisson distribution this squared width will decrease as $1/N^{\mathrm{eq}}$. We plot $\sqrt{W_{ii}}$ in Fig. 3 for an ideal gas, a real dilute gas, and a dense gas as a function of the number of average number particles per lattice site. The dilute gas results agree quite well with a Poisson distribution up to about 1000 particles per lattice site. After that the width fails to decrease as fast as expected for an ideal gas. This agrees with the results in Fig. 1.

For the dense gas the scaled width of the distribution diverges from the ideal gas case at about 10 particles per lattice site, and decays much more slowly for larger numbers of particles. This implies that the importance of fluctuations does no longer decay as $1/\sqrt{N^{\mathrm{eq}}}$. Therefore, increasing the coarse graining by choosing a larger lattice spacing Δx will not diminish fluctuations as rapidly as would be expected in standard statistical mechanics. The difference is striking: instead of decaying as $(N^{\mathrm{eq}})^{-1/2}$, the rest particles scale approximately as $(N^{\mathrm{eq}})^{-1/4}$, and moving particle density only as $(N^{\mathrm{eq}})^{-1/8}$. This result may seem counterintuitive: basic statistical mechanics would seem to demand that if we continue to double the lattice spacing Δx, the added components should eventually become independent. This argument, however, misses the important point

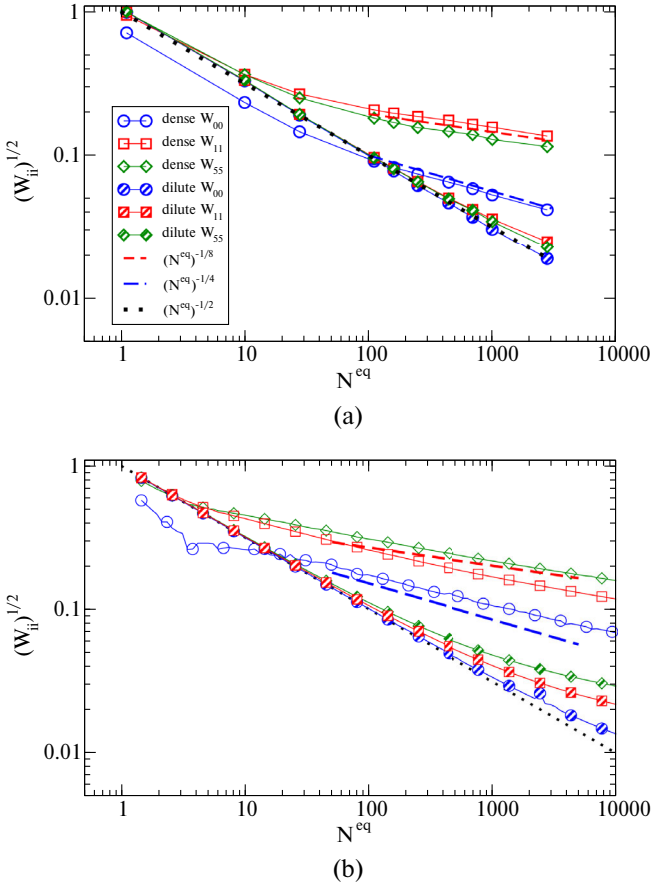

FIG. 3. Scaled distributions compared to that of a Poisson distribution for the MDLG system (a) and a theoretical prediction from the simplified two-particle displacement probability of Eq. (16) (b). For larger coarse graining the width of the distributions can be orders of magnitude wider than expected for an ideal gas. This transition is enhanced for denser systems, but appears for all densities. The theoretical result obtained by numerical evaluation with *Mathematica* shows some numerical wiggles, indicating that the software has some difficulties evaluating the required four-dimensional integral.

that we are keeping $a^2 = 1/6$, so that the time step Δt also increases.

Let us consider the probability of the particle displacements. Instantaneous velocities in equilibrium remain uncorrelated,

$$P^2(x_1, v_1, x_2, v_2) \propto P(v_1)P(v_2)g(|x_1 - x_2|), \quad (13)$$

where $g(r)$ is the pair correlation function. The same is not true for displacement probabilities $P_2(x_k, \delta_k, x_l, \delta_l)$. Displacements $\delta_k = \int_0^{\Delta t} v_k(t)dt$ are not independent because they depend on velocities at different times. For particles sufficiently far apart, the displacement probability will factorize:

$$\lim_{|x_2 - x_1| \to \infty} P^2(x_1, \delta_1, x_2, \delta_2) = P^1(x_1, \delta_1)P^1(x_2, \delta_2). \quad (14)$$

It is well known that, particularly for longer times, the time correlator for velocities decays only algebraically [30]. It is reasonable to expect a similar effect for velocities of particles that have a small spatial separation. A comprehensive numerical evaluation of these correlations is outside the scope of this Letter, but we did examine $\langle \delta_1 \delta_2 \rangle$ as a function of the initial displacement of the particles $|x_2 - x_1|$ [31]. We found that this correlator does appear to decay exponentially with a correlation length $\xi \approx \langle \delta^2 \rangle$ with a prefactor that varies remarkably little with density (from 1 to 1.25 for the two extreme densities studied in this Letter).

As shown in the Supplemental Material [29], the approximate relation

$$\frac{\langle \delta_1 \delta_2 \rangle (|x_1 - x_2|)}{\langle \delta_1^2 \rangle} \approx 2 \left(\frac{N^{\mathrm{eq}}}{\Delta x} \right)^{1/2} \exp\left(-\frac{|x_1 - x_2|}{\xi \Delta x} \right) \quad (15)$$

holds where ξ now varies slightly from 1 to 1.25 for our density range. There are two caveats to this approximate result. Firstly, at short distances the normalized correlation of Eq. (15) has to be less than one. Secondly, the total expectation of $\langle \delta_1 \delta_2 \rangle = 0$ because of momentum conservation. In numerical experiments we find that for large Δx there is actually a negative correlation, but the value of this correlation function for large Δx is not of interest here. Even with these caveats this result implies that the nonideal part of the two-particle probability also decays exponentially with correlation length ξ. We can now make the following ansatz that will recover both the factorization of Eq. (13) and the correlation of Eq. (15):

$$P(x_1, \delta_1, x_2, \delta_2) \propto g(r) \exp\left(-\frac{(\delta_1 + \delta_2)^2}{4\sigma_+^2(r)} \right) \exp\left(-\frac{(\delta_1 - \delta_2)^2}{4\sigma_-^2(r)} \right), \quad (16)$$

where $r = |x_1 - x_2|$ and

$$\sigma_\pm(r) = a\Delta x \sqrt{1 \pm \langle \delta_1 \delta_2 \rangle (r) / \langle \delta_1 \delta_1 \rangle}. \quad (17)$$

This is the simplest two-particle distribution function that recovers both Eq. (14) and Eq. (15). We use numerical integration to estimate the occupation number correlators in Eq. (10). The numerical integration was performed using *Mathematica*, using the rough two-particle correlation function,

$$g(r) = \frac{1}{2} \tanh\left(\frac{|x_1 - x_2| - r_c}{0.03} \right) + \frac{1}{2}, \quad (18)$$

and a *Mathematica* notebook is included in the Supplemental Material [29]. The results of this numerical integration are shown in Fig. 3, and it qualitatively recovers the result of the direct simulations.

In conclusion, we have found that apparent equal-time fluctuations in coarse-grained models contain time correlations, which can significantly alter the scaling of the fluctuations. It is well known that while equal-time fluctuations in equilibrium systems decay exponentially, different-time fluctuations only decay algebraically [30], so that the contribution of different-time correlations can be significant. This does not change the short-ranged nature of these fluctuations, as can be seen in Eq. (15). But the magnitude of fluctuations can be orders of magnitude larger for the coarse-grained system variables when compared to quantities that are obtained from equal-time correlators like density or momentum fluctuations. This property of mesoscopic methods has not been fully appreciated to date. A long history of previous lattice gas approaches made a Markov approximation, which implies that occupation numbers were viewed as instantaneous quantities. Such a view is in contrast to our lattice gas, which is a true coarse graining of reality, as represented by a MD simulation, and has fundamentally different properties. This interpretation of a lattice gas as a coarse-grained model represents a shift in perception, and we believe that our results will facilitate the development of more realistic coarse-grained fluctuating methods.

Lastly, we would like to emphasize that the large fluctuations observed in this Letter should not be thought of as restricted to lattice gas approaches, but that these will appear in all coarse-grained approaches, like those mentioned in the introduction.

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