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Monte Carlo Simulation of Phase Transitions in Three-Dimensional Quantum Lattice Models*

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Using quantum Monte Carlo techniques recently developed [1], we have studied the thermodynamic properties of a model of interacting bosons on a three-dimensional spatial lattice. The proposed model [2] is interesting in that it exhibits gas, liquid, and solid-like phases together with an assortment of first-order and second-order phase transitions. The structure of the resulting phase diagram, in many ways, resembles that of He^4 at low temperatures. The Hamiltonian for the system is taken to be

$$\mathcal{H} = \frac{1}{2}\sum_{<i,j>}(\psi_i^+ - \psi_j^+)(\psi_i - \psi_j) - v\sum_{<i,j>}\hat{n}_i\hat{n}_j + w\sum_{<i,j,k>}\hat{n}_i\hat{n}_j\hat{n}_k$$

where the sites i form a cubic lattice with periodic boundary conditions and where the boson field operators ψ_i are related to the site occupation number operators $\hat{n}_i$ according to $\hat{n}_i = \psi_i^+\psi_i$. To effect a hard-core repulsion, we restrict the occupation numbers to be 0 or 1. The v-term ($v > 0$) represents nearest neighbor attractions; while the w-term ($w > 0$) represents three-body repulsions for bosons located on three adjacent colinear sites. This latter term is included so as to break the symmetry between $\hat{n}_i$ and $(1 - \hat{n}_i)$.

The model for $w = 0$ is actually equivalent to the anisotropic Heisenberg spin model and has been studied in mean field theory by Matsubara and Matsuda [3] and by Zilsel [4]. Their studies indicate: (1) for $v < 1$, first-order transitions are not present but two distinct second-order transitions do occur at each temperature below $kT_\lambda = 1.5$; and (2) for $v > 1$, second-order transitions are not present but a single first-order transition does occur at each temperature below $kT_c = 1.5v$. In fact, we have carried out extensive Monte Carlo simulations [5] of the anisotropic Heisenberg model and have found these mean field theory results to be qualitatively correct (although the simulation's values for kT_λ and kT_c are substantially lower than the mean field values). The conclusion that the phase diagram for fixed v contains either first-order or second-order transitions, but not both, stems from the Heisenberg model's symmetry between low density ($n_i < \frac{1}{2}$) and high density ($n_i > \frac{1}{2}$). Our introduction of a three-body interaction is a particularly simple way to break this symmetry and permit a much more elaborate phase structure.

Our mean field theory analysis for the case $w \neq 0$ suggests that the model has a rich phase diagram with both first-order and second-order transitions occurring among gas, liquid, and solid-like phases. For $v > 1$ and w small

compared to v, solid-like phases are absent but gas and liquid phases separated by a first-order transition are present. In addition, a second-order transition line separates two distinct phases of the liquid. For large values of w, solid-like phases emerge at high densities. Preliminary results of our simulation studies indicate that, once again, the mean field theory predictions are qualitatively correct.

The Monte Carlo method we use replaces the original quantum problem on a three-dimensional L^3 lattice by an equivalent classical problem on a four-dimensional $L^3 \times M$ lattice, where M denotes the number of "time slices" [1, 6, 7]. The effects of using finite L and finite M have been examined by considering different size lattices with $L = 8, 12, 16$ and $M = 12, 24, 48$. For example, the thermodynamic quantities we compute have the form $A+BM^{-2}$ for large M, so that the required $M \rightarrow \infty$ limit can easily be extrapolated. The simulations have been done primarily in the grand canonical ensemble.

The evidence for a first-order transition comes from measuring the average number of particles $<N>$ as a function of chemical potential μ and observing a significant jump in $<N>$ in the vicinity of some critical value of μ. Moreover, at this critical μ, the sweep-by-sweep time evolution of the number of particles in the system indicates the coexistence of two distinct phases having very different number densities. Figure 1 (for $v = 2.0$ and $w = 0.0$) and figure 2 (for $v = 6.0$ and $w = 2.7$) depict such a two-phase coexistence.

At a second-order transition, the fluctuation in the particle number as a function of $<N>$ has a maximum, the height of which increases as the spatial volume L^3 is made larger. Figure 3 (for $v = 0.5$ and $w = 0.0$) clearly indicates such second-order behavior at one low-density value as well as at the symmetrically-located high density value, when kT equals 0.7. In contrast, the relatively smooth behavior in figure 4 (also for $v = 0.5$ and $w = 0.0$) shows that the second-order transition has disappeared when kT has been increased to 1.0. One should note that the first-order transition of figure 1 and the second-order transitions of figure 3 necessarily occur for different values of the parameter v with $w = 0$. Figures 5 and 6 (both for $v = 6.0$ and $w = 2.7$) give preliminary indications of a high-density second-order transition at low temperature ($kT = 0.4$) and the absence of such a transition at high temperature ($kT = 0.8$). One should note that the first-order transition of figure 2 and the second-order transition of figure 5 occur for the *same* value of the parameter v and the *same* non-zero w.

Our preliminary simulation results for the lattice model with $v = 6.0$ and $w = 2.7$ can be summarized in the phase diagram of figure 7. The axes of this diagram indicate temperature and average number density. A first-order transition line (full line) separates a pure phase from a coexistence region, while a second-order transition line (broken line) serves as the boundary between two contiguous phases. The simulation results (data points with connecting lines as a guide for the eye) are shown together with the mean field theory predictions.

For sufficiently larger values of w, mean field theory suggests the existence of additional transitions to solid-like phases. We have searched for such solids by measuring the site-number correlation $<\hat{n}_i\hat{n}_j>$ as a function of the separation between sites i and j. Figures 8 and 9 (both for $v = 6.0$ and $w = 4.0$) show results for $kT = 1.0$ and 4.0, respectively. The periodic structure at the low temperature of figure 8 indicates the formation of a solid-like phase. At the higher temperature of figure 9, the periodicity is absent and the correlation function has the behavior typical of a liquid.

We are now beginning a systematic survey of the thermodynamic properties of our model over a large range of v and w values. The rich assortment of phases with their first-order and second-order transitions when w is non-zero makes this an interesting model to study.

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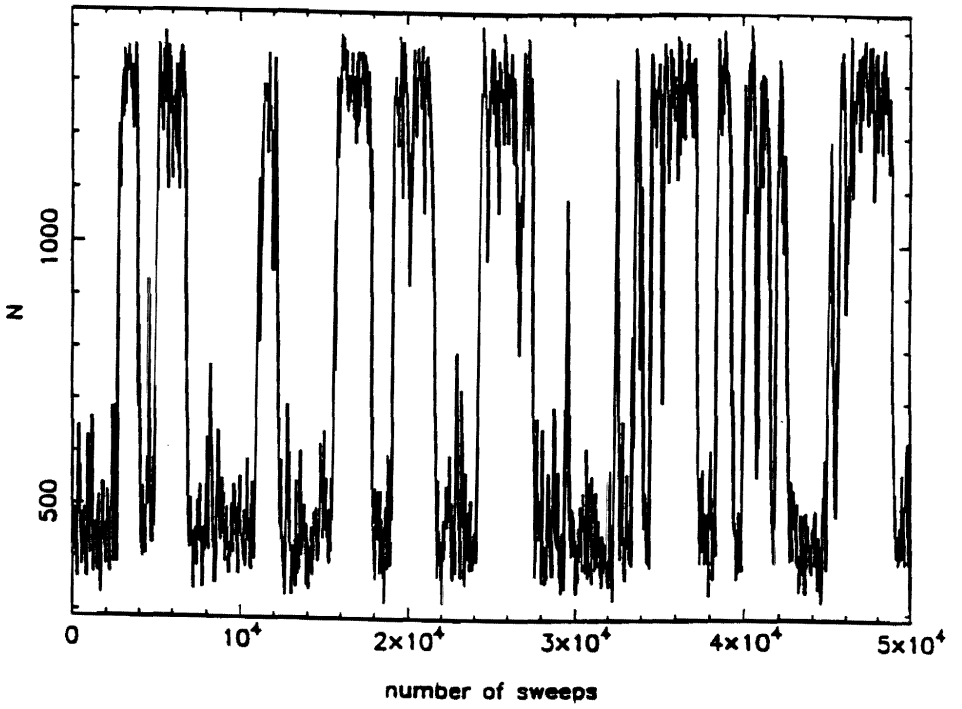

Fig. 1. The time evolution of particle number in a MC run showing the coexistence of gas and liquid phases for a $12^3 \times 12$ lattice, $v = 2.0$, $w = 0.0$, $kT = 2.1$, and $\mu = -3.0$.

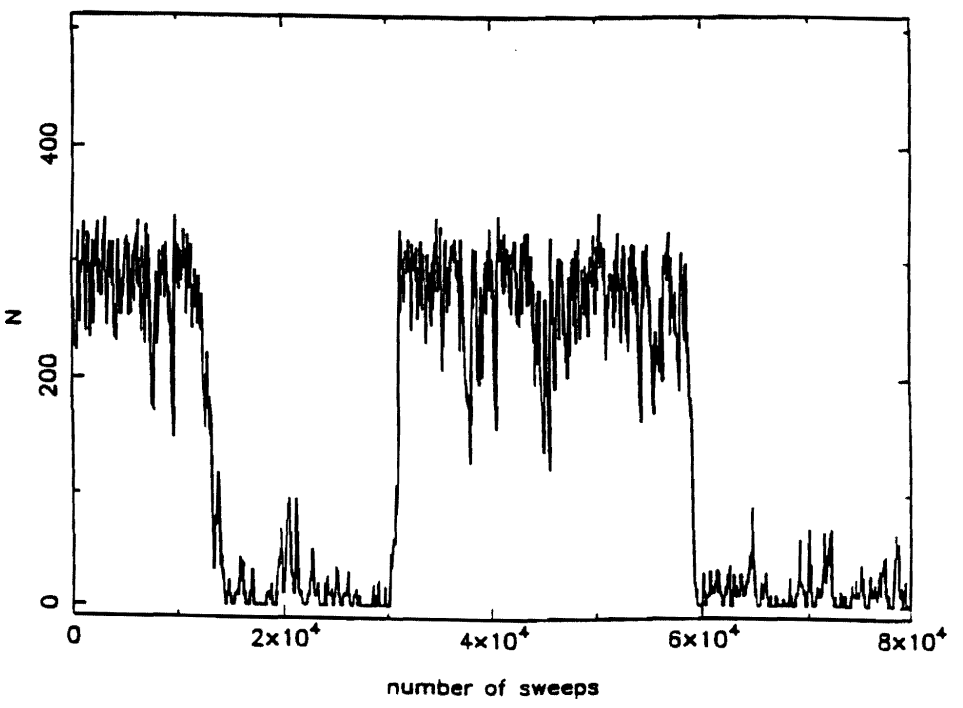

Fig. 2. The time evolution of particle number in a MC run showing the coexistence of gas and liquid phases for an $8^3 \times 12$ lattice, $v = 6.0$, $w = 2.7$, $kT = 1.5$, and $\mu = -7.56$.

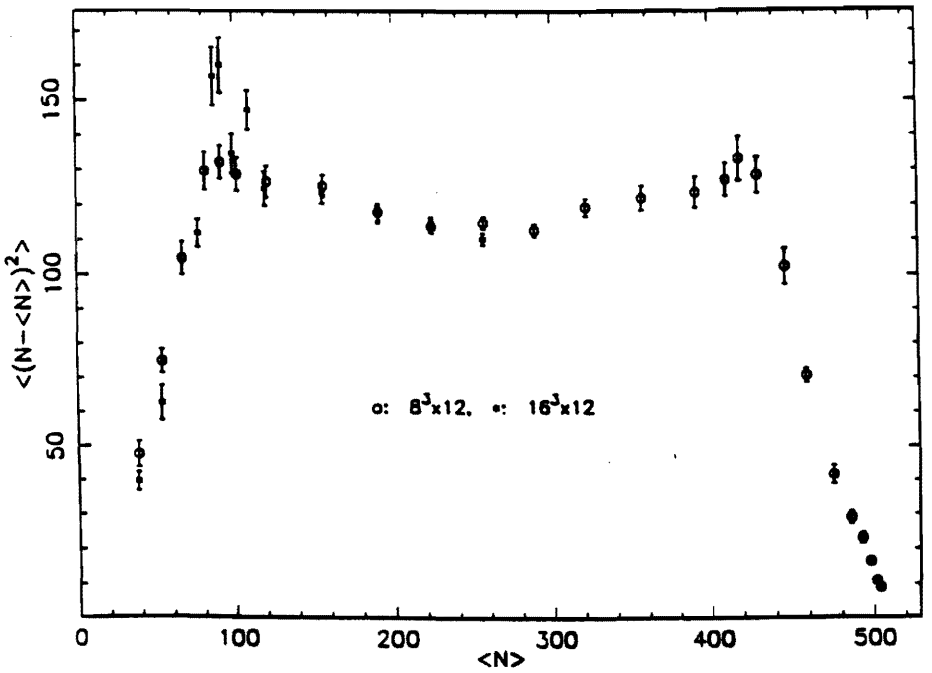

Fig. 3. The particle number fluctuation plotted against the average particle number. The two peaks indicate the presence of two second-order transitions. The data are for $8^3 \times 12$ and $16^3 \times 12$ lattices, $v = 0.5$, $w = 0.0$, and $kT = 0.7$.

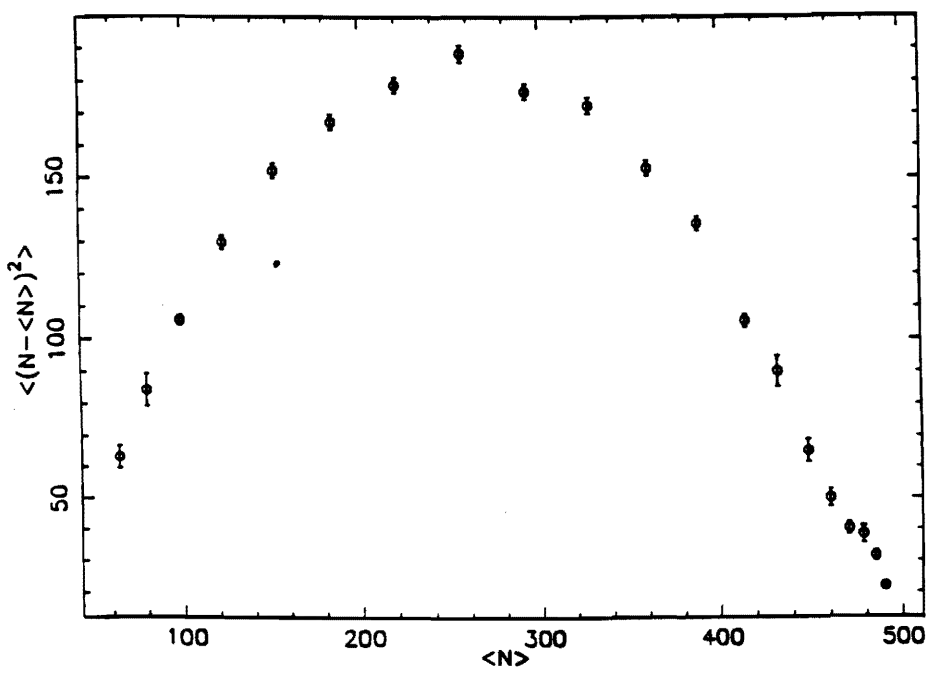

Fig. 4. The particle number fluctuation plotted against the average particle number. The smooth behavior indicates the absence of any second-order phase transition. The data are for an $8^3 \times 12$ lattice, $v = 0.5$, $w = 0.0$, and $kT = 1.0$.

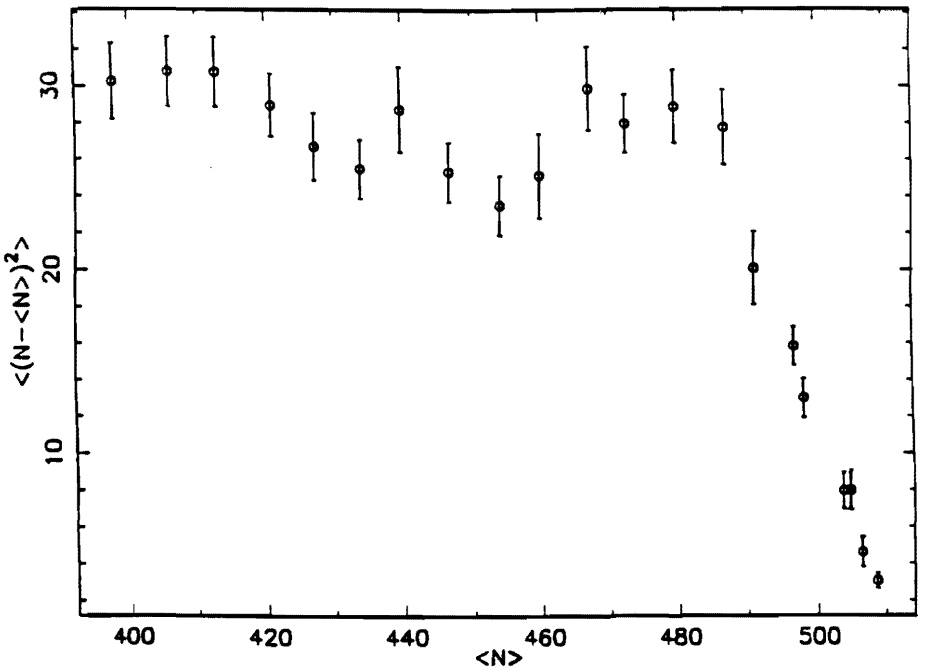

Fig. 5. The particle number fluctuation plotted against the average particle number. There is preliminary evidence for a second-order transition at $\langle N \rangle \approx 480$. The data are for an $8^3 \times 24$ lattice, $v = 6.0$, $w = 2.7$, and $kT = 0.4$.

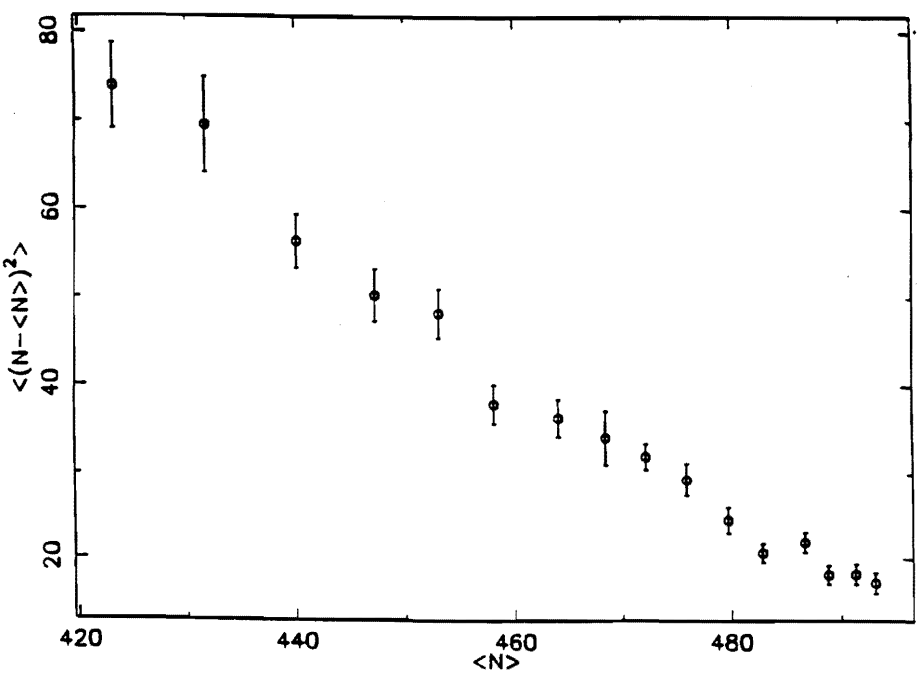

Fig. 6. The particle number fluctuation plotted against the average particle number. The smooth behavior indicates the absence of any second-order phase transition. The data are for an $8^3 \times 12$ lattice, $v = 6.0$, $w = 2.7$, and $kT = 0.8$.

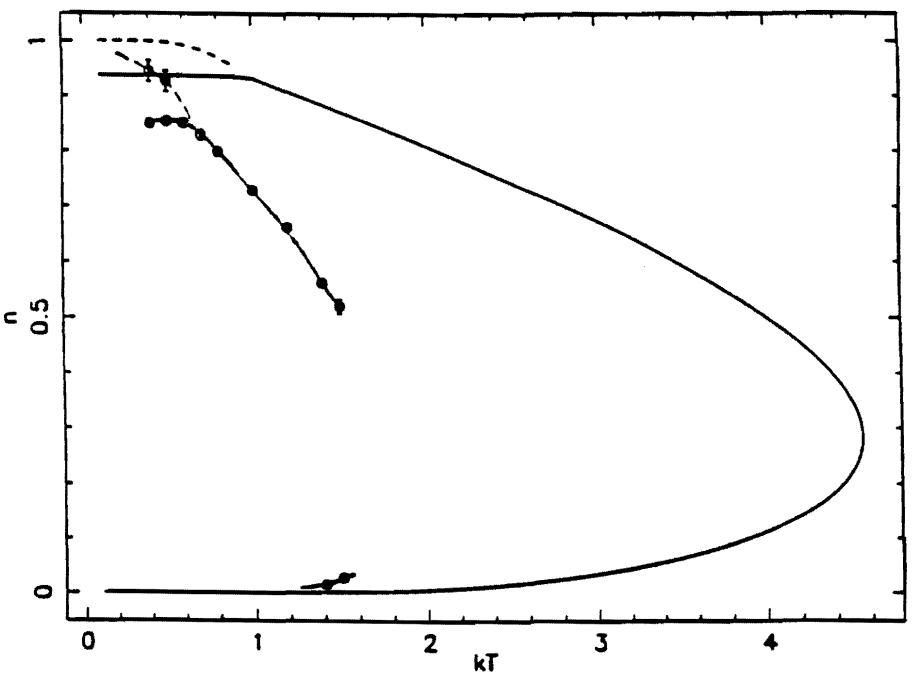

Fig. 7. The phase diagram for $v = 6.0$ and $w = 2.7$ from MC simulation and mean field theory. The first-order line (full line) separates a pure phase from a coexistence region, while a second-order line (broken line) separates the two contiguous phases. The simulation results (data points with connecting lines as a guide for the eye) are shown together with the mean field theory predictions.

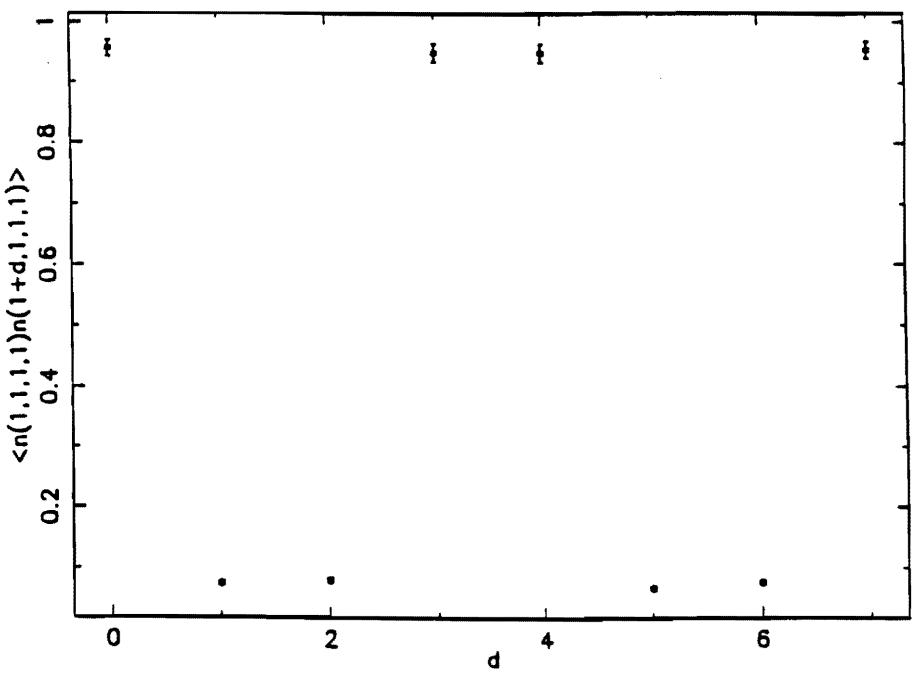

Fig. 8. Correlation function for a solid-like phase for an $8^3 \times 12$ lattice, $v = 6.0$, $w = 4.0$, $kT = 1.0$, and $n = 0.53$.

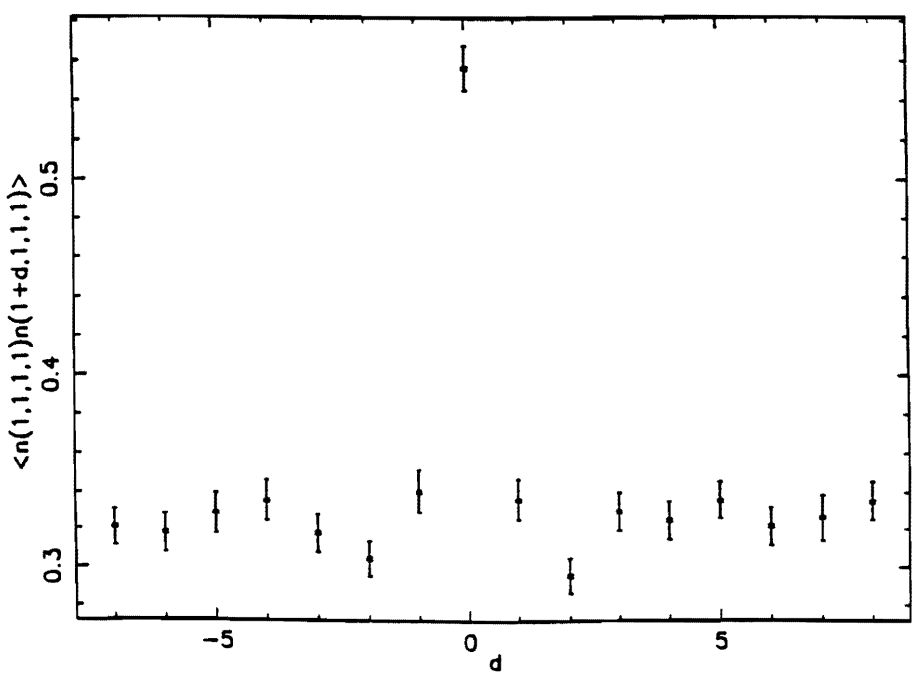

Fig. 9. Correlation function for a fluid phase for a $16^3 \times 12$ lattice, $v = 6.0$, $w = 4.0$, $kT = 4.0$, and $n = 0.58$.