Monte Carlo studies of three-dimensional O(1) and O(4) ϕ^4 theory related to Bose-Einstein condensation phase transition temperatures

Xuepeng Sun
Department of Physics, University of Virginia, P.O. Box 400714, Charlottesville, Virginia 22904-4714, USA
(Received 7 August 2002; published 9 June 2003)

The phase transition temperature for the Bose-Einstein condensation (BEC) of weakly interacting Bose gases in three dimensions is known to be related to certain nonuniversal properties of the phase transition of three-dimensional O(2) symmetric ϕ^4 theory. These properties have been measured previously in Monte Carlo lattice simulations. They have also been approximated analytically, with moderate success, by large N approximations to O(N) symmetric ϕ^4 theory. To begin investigating the region of validity of the large N approximation in this application, the same Monte Carlo technique developed for the O(2) model [P. Arnold and G. Moore, Phys. Rev. E **64**, 066113 (2001)] to O(1) and O(4) theories has been applied. The results indicate that there might exist some theoretically unanticipated systematic errors in the extrapolation of the continuum value from lattice Monte Carlo results. The final results show that the difference between simulations and next-to-leading order large N calculations does not improve significantly from $N=2$ to $N=4$. This suggests that one would need to simulate yet larger N's to see true large N scaling of the difference. Quite unexpectedly (and presumably accidentally), the Monte Carlo result for $N=1$ seems to give the best agreement with the large N approximation among the three cases.

DOI: 10.1103/PhysRevE.67.066702 PACS number(s): 02.70.Uu, 64.60.−i

I. INTRODUCTION

The computation of the phase transition temperature T_c for dilute or weakly interacting Bose gases has attracted considerable interest. Due to the nonperturbative nature of long-distance fluctuations at the second-order phase transition at large distance, the calculation of corrections to the ideal gas formula for T_c is nontrivial. In the dilute or weakly interacting limit, the correction $\Delta T_c \equiv T_c - T_0$ to the ideal gas result T_0 for a homogeneous gas can be parametrized as[1]

$$\frac{\Delta T_c}{T_0} = c a_{\rm sc} n^{1/3} + O(a_{\rm sc}^2 n^{2/3} \ln(a_{\rm sc} n^{1/3})), \tag{1.1}$$

where a_{sc} is the scattering length of the two-particle interaction, n is the number density of the homogeneous gas, c is a numerical constant, and $O(\cdots)$ shows the parametric size of higher-order corrections. Baym *et al.* [1] have shown that the computation of c can be reduced to a problem in three-dimensional O(2) ϕ^4 field theory. In general, O(N) ϕ^4 field theory is described by the continuum action

$$S_{\rm cont} = \int d^3x \left[\frac{1}{2} (\nabla \phi)^2 + \frac{1}{2} r \phi^2 + \frac{u}{4!} (\phi^2)^2 \right], \tag{1.2}$$

where $\phi = (\phi_1, \phi_2, \ldots, \phi_N)$ is an N-component real field. I will focus exclusively on the case where r has been adjusted to be at the order or disorder phase transition for this theory for a given value of the quartic coupling u. The relationship to T_c for the Bose-Einstein condensation found by Baym *et al.* is that the constant c in Eq. (1.1) is[2]

$$c = - \frac{128 \pi^3}{\left[\zeta\left(\frac{3}{2}\right) \right]^{4/3}} \frac{\Delta \langle \phi^2 \rangle_c}{u}, \tag{1.3}$$

where $\phi^2 \equiv \phi_1^2 + \phi_2^2 + \cdots \phi_N^2$, $N=2$ and

$$\Delta \langle \phi^2 \rangle_c \equiv [\langle \phi^2 \rangle_c]_u - [\langle \phi^2 \rangle_c]_0 \tag{1.4}$$

represents the difference between the critical-point value of $\langle \phi^2 \rangle$ for the cases of (i) u being nonzero and (ii) the ideal gas $u=0$. Thus, the computation of the first correction to T_c due to interactions is related to the evaluation of $\Delta \langle \phi^2 \rangle_c$ in three-dimensional ϕ^4 theory.

Having tuned r to the phase transition, u is then the single remaining parameter of the three-dimensional continuum ϕ^4 theory (1.2). The dependence of (ultraviolet-convergent) quantities on u is determined by simple dimensional analysis, and u has dimensions of inverse length. The $\Delta \langle \phi^2 \rangle_c / u$ in Eq. (1.3) is dimensionless and so is a number independent of u in the continuum theory. Monte Carlo simulations of this quantity in O(2) theory have given $c = 1.29 \pm 0.05$ [4] and $c = 1.32 \pm 0.02$ [5].

One of the few moderately successful attempts to approximate this result with an analytic calculation has been through the use of the large N approximation. (But see also the fourth-order linear δ expansion results of Refs. [7]. For a brief comparison of the results of a wide spread of attempts to estimate c, see the introduction to Ref. [6] and also Ref.

[1]For a clean argument that the first correction is linear in $a_{\rm sc}$, see Ref. [1]. For a discussion of higher-order corrections, see Refs. [2,3].

[2]This is given separately in Ref. [1] as $\Delta T_c / T_0 = -2 m k_B T_0 \Delta \langle \phi^2 \rangle_c / 3 \hbar^2 n$ and the identification of u as $96 \pi^2 a_{\rm sc} / \lambda^2$.

TABLE I. Simulation results for $N=1,2,4$ and the NLO large N results for $\Delta\langle\phi^2\rangle_c/u$. The difference column shows the percentage excess of the magnitude of the large N approximation result over the magnitude of the simulation result. $N=2$ simulation results are quoted from Ref. [5].

	$\Delta\langle\phi^2\rangle_c/u$			$r_c/u^2(\bar{\mu}=u/3)$
N	Simulation	Large N	Difference	Simulation
1	−0.000494(41)	−0.0004990	−1(8)%	0.0015249(48)
2 (Ref. [5])	−0.001198(17)	−0.001554	+30(2)%	0.0019201(21)
4	−0.00289(18)	−0.003665	+27(8)%	0.002558(16)

[8].) The procedure is to calculate $\Delta\langle\phi^2\rangle_c/u$ for O(N) theory in the limit where N is arbitrarily large, and then substitute the actual value $N=2$ of interest into the result. The large N result was originally computed at leading order in $1/N$ by Baym, Blaizot, and Zinn-Justin [9] and was extended to next-to-leading order (NLO) in $1/N$ by Arnold and Tomášik [10], giving[3]

$$\frac{\Delta\langle\phi^2\rangle_c}{u}=-\frac{N}{96\pi^2}\left[1-\frac{0.527\,198}{N}+O(N^{-2})\right]. \quad (1.5)$$

Setting $N=2$, one obtains $c\sim 1.71$, which is roughly 30% higher than the results obtained by the Monte Carlo simulation of O(2) theory. Considering that $N=2$ has been treated as large in this approximation, the result is fairly encouraging.

The goal of the present work is to further explore the applicability of the large N result (1.5) by testing it for other values of N. I have applied to other O(N) models the same techniques used in Ref. [5] to simulate the O(2) model. In this paper, I report the measurement of $\Delta\langle\phi^2\rangle_c/u$ for the O(1) and O(4) theories. The final results, compared to the large N approximations of Eq. (1.5), are given in Table I.

As a byproduct of the analysis, I also report the measurement of the critical value r_c of r. The coefficient r requires ultraviolet renormalization and so is convention dependent. In Table I, I report the dimensionless continuum values of r_c/u^2 with r_c being defined by dimensional regularization and modified minimal subtraction ($\overline{\rm MS}$) renormalization at a renormalization scale $\bar{\mu}$ set to $u/3$. Among other things, this quantity can be related to the coefficient of the second-order ($a_{\rm sc}^2 n^{2/3}$) correction to ΔT_c [2,11]. One can convert to other choices of the $\overline{\rm MS}$ renormalization scale $\bar{\mu}$ by the (exact) identity

$$\frac{r^{\overline{\rm MS}}(\bar{\mu}_1)}{u^2}=\frac{r^{\overline{\rm MS}}(\bar{\mu}_2)}{u^2}+\frac{(N+2)}{18(4\pi)^2}\ln\frac{\bar{\mu}_1}{\bar{\mu}_2}. \quad (1.6)$$

In Sec. II, I briefly review the algorithm and the necessary background materials and formulas for improving the extrapolations of the continuum and infinite-volume limits. Most of the technical details can be found in Ref. [5]. Section III gives the simulation results and analysis. Section IV is the conclusion from comparing the numerical results with the NLO large N calculation (1.5).

II. LATTICE ACTION AND METHODS

The action of the theory on the lattice is given by

$$S_{lat}=a^3\sum_x\left\{\frac{1}{2}\Phi_{\rm lat}(-\nabla^2_{\rm lat})\Phi_{\rm lat}+\frac{1}{2}r_0\Phi^2_{\rm lat}+\frac{u_0}{4!}(\Phi^2_{\rm lat})^2\right\}, \quad (2.1)$$

where a is the lattice size (not to be confused with the scattering length $a_{\rm sc}$). I will work on simple cubic lattices with cubic total volumes and periodic boundary conditions. As in Ref. [5] and as reviewed further below, the bare lattice operators and couplings ($\Phi_{\rm lat},\Phi^2_{\rm lat},r_0,u_0$) are matched to the continuum, using results from lattice perturbation theory to improve the approach to the continuum limit for finite but small lattice spacing.

I shall use the improved lattice Laplacian

$$\nabla^2\Phi(\mathbf{x})=a^{-2}\sum_{\mathbf{i}}\left[-\frac{1}{12}\Phi(\mathbf{x}+2a\mathbf{i})+\frac{4}{3}\Phi(\mathbf{x}+a\mathbf{i})-\frac{5}{2}\Phi(\mathbf{x})+\frac{4}{3}\Phi(\mathbf{x}-a\mathbf{i})-\frac{1}{12}\Phi(\mathbf{x}-2a\mathbf{i})\right], \quad (2.2)$$

which (by itself) has $O(a^4)$ errors, rather than the standard unimproved Laplacian

$$\nabla^2_U\Phi(\mathbf{x})=a^{-2}\sum_{\mathbf{i}}\left[\Phi(\mathbf{x}+a\mathbf{i})-2\Phi(\mathbf{x})+\Phi(\mathbf{x}-a\mathbf{i})\right], \quad (2.3)$$

which has $O(a^2)$ errors. Readers interested in simulation results with the unimproved kinetic term should see Ref. [23].

Because the only parameter of the continuum theory (1.2) at its phase transition is u, the relevant distance scale for the

[3]If combining Eqs. (1.3) and (1.5), note that Eq. (1.3) only applies in the case $N=2$, which corresponds to a single-component ideal gas. Alternatively, as a theoretical excercise, one could imagine a gas where each boson had a degenerate set of $N/2$ internal quantum states with $U(N/2)$ symmetry for any even N. In this case, T_0 would be proportional to N, and Eq. (1.3) should have an additional factor of $2/N$ on the right-hand side. This factor of $1/N$ in Eq. (1.3) would cancel the overall factor of N in Eq. (1.3) when the two are combined.

physics of interest is of order $1/u$ by dimensional analysis. To approximate the continuum infinite-volume limit, one needs lattices with total linear size L, large compared to this scale and lattice spacing a small compared to this scale. As a result, ua is the relevant dimensionless expansion parameter for perturbative matching calculations intended to eliminate lattice spacing errors to some order in a. The analogous dimensionless parameter that will appear in the later discussions of the large volume limit is Lu.

A. Matching to continuum parameters

To account for the lattice spacing errors, I have adapted the perturbative matching calculations to improve lattice spacing errors given in Ref. [5], where the details of the calculations can be found. Here I will simply collect the results from that reference. The lattice action expressed in terms of continuum parameters is written in the form

$$S_{\rm lat}\equiv a^3\sum_x \left\{ \frac{Z_\phi}{2}(\nabla_{\rm lat}\phi)^2+\frac{Z_r}{2}(r+\delta r)\phi^2+\frac{u+\delta u}{4!}(\phi^2)^2\right\}. \tag{2.4}$$

The continuum approximate value for $\Delta\langle\phi^2\rangle_c$ is theoretically expected to have the form

$$\Delta\langle\phi^2\rangle_c = Z_r\langle\phi^2\rangle_{\rm lat}-\delta\phi^2+O(a^2). \tag{2.5}$$

For the improved Laplacian, the matching calculations have been done to two-loop level ($2l$) for Z_ϕ, Z_r, δr, and δu, and three loops ($3l$) for $\delta\phi^2$, yielding

$$\delta\phi^2_{3l}=\frac{N\Sigma}{4\pi a}+\frac{N(N+2)}{6}\frac{\Sigma\xi}{(4\pi)^2}u-\frac{\xi}{4\pi}Nra + \left[\left(\frac{N+2}{6}\right)^2\xi^2\Sigma+\frac{(N+2)}{18}[C_4-3\Sigma C_1-\Sigma C_2 + \xi\ln(a\bar{\mu})]\right]\frac{Nu^2a}{(4\pi)^3}, \tag{2.6a}$$

$$\delta u_{2l}=\frac{(N+8)}{6}\frac{\xi}{4\pi}u^2a+\left[\frac{(N^2+6N+20)}{36}\left(\frac{\xi}{4\pi}\right)^2 - \frac{(5N+22)}{9}\frac{C_1}{(4\pi)^2}\right]u^3a^2, \tag{2.6b}$$

$$Z_{\phi,2l}=1+\frac{(N+2)}{18}\frac{C_2}{(4\pi)^2}u^2a^2, \tag{2.6c}$$

$$Z_{r,2l}=1+\frac{(N+2)}{6}\frac{\xi}{4\pi}ua+\left[\left(\frac{N+2}{6}\right)^2\left(\frac{\xi}{4\pi}\right)^2 - \frac{(N+2)}{6}\frac{C_1}{(4\pi)^2}\right](ua)^2, \tag{2.6d}$$

$$\delta r_{2l}=-\frac{(N+2)}{6}\frac{\Sigma}{4\pi}ua+\frac{(N+2)}{18(4\pi)^2}\left[C_3+\ln\left(\frac{6}{\bar{\mu}}\right)-3\Sigma\xi\right] \times(ua)^2, \tag{2.6e}$$

where, for the improved Laplacian (2.2),

$$\Sigma\simeq 2.75238391130752, \tag{2.7a}$$

$$\xi\simeq -0.083647053040968, \tag{2.7b}$$

$$C_1\simeq 0.0550612, \tag{2.7c}$$

$$C_2\simeq 0.03344161, \tag{2.7d}$$

$$C_3\simeq -0.86147916, \tag{2.7e}$$

$$C_4\simeq 0.282. \tag{2.7f}$$

As shown in Ref. [5], the result of this improvement is that at fixed physical system size Lu, the lattice spacing error of $\Delta\langle\phi^2\rangle_c/u$ should be $O(a^2)$. However, as will be shown in the following, my simulation results indicate that there might still exist some linear coefficients even after applying formula (2.5). I assign an error to my continuum extrapolations that covers both linear and quadratic extrapolations.

This has produced about 10% systematic error in the final value of $\Delta\langle\phi^2\rangle_c/u$. The extrapolation of r_c/u^2 on the other hand has $O(a)$ error, since no improvement has been made. Overall, the fitting formulas for the data taken at fixed Lu are given as

$$\left\{\frac{\Delta\langle\phi^2\rangle_c}{u}\right\}_{Lu}=B_1+B_2(ua)^2, \tag{2.8a}$$

$$\left\{\frac{r_c}{u^2}\right\}_{Lu}=D_1+D_2(ua), \tag{2.8b}$$

for a quadratic fit of $\Delta\langle\phi^2\rangle_c/u$, and

$$\left\{\frac{\Delta\langle\phi^2\rangle_c}{u}\right\}_{Lu}=B_1+B_2'(ua), \tag{2.9a}$$

$$\left\{\frac{r_c}{u^2}\right\}_{Lu}=D_1+D_2(ua), \tag{2.9b}$$

for a linear fit of $\Delta\langle\phi^2\rangle_c/u$.

B. Algorithm and finite-volume scaling

Working in lattice units ($a=1$) with the lattice action (2.4), I update the system by heat bath and multigrid methods [21]. At each level of the multigrid update, I perform overrelaxation updates. Statistical errors are computed using the standard jackknife method.

The strategy is to vary r at fixed u to reach the phase transition point. In order to define a nominal ''phase transition'' point in a finite volume, I use the method of Binder

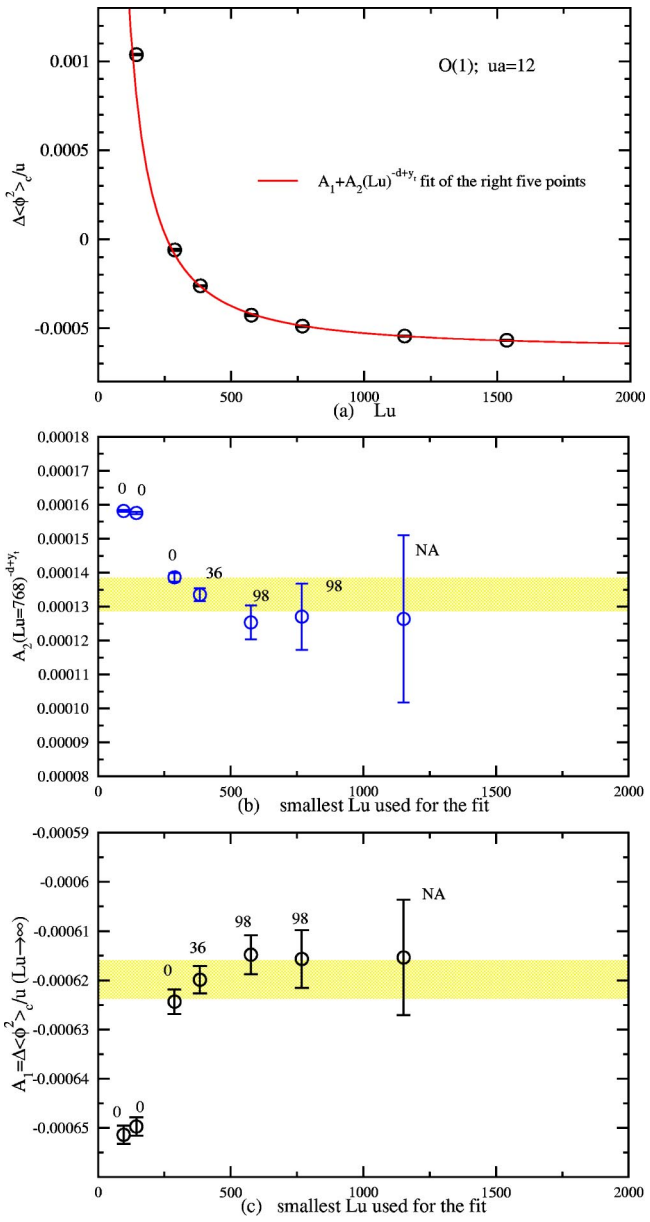

FIG. 1. (a) Shows the simulation result for $\Delta\langle\phi^2\rangle_c/u$ vs physical volume at $ua=12$ for O(1); (b) is the result of the difference between the (768,12)* point and the infinite extrapolation; (c) is the $Lu\to\infty$ extrapolations; and since we used the fitting formula for $\Delta\langle\phi^2\rangle_c/u$ at (768,12)* (2.5), this difference depends only on the results of A_2 but not on A_1. In both (b) and (c), the shaded areas are the quoted results. The confidence levels are given as the percentage numbers on top of the fitted values. "NA" stands for "nonapplicable," which means the number of the fitting parameters equals the number of fitted points. The numbers shown in all graphs and tables are dimensionless.

cumulants [22]. The Binder cumulant of interest is defined by

$$C=\frac{\langle\bar{\phi}^4\rangle}{\langle\bar{\phi}^2\rangle^2}, \tag{2.10}$$

where $\bar{\phi}$ is the volume average of ϕ,

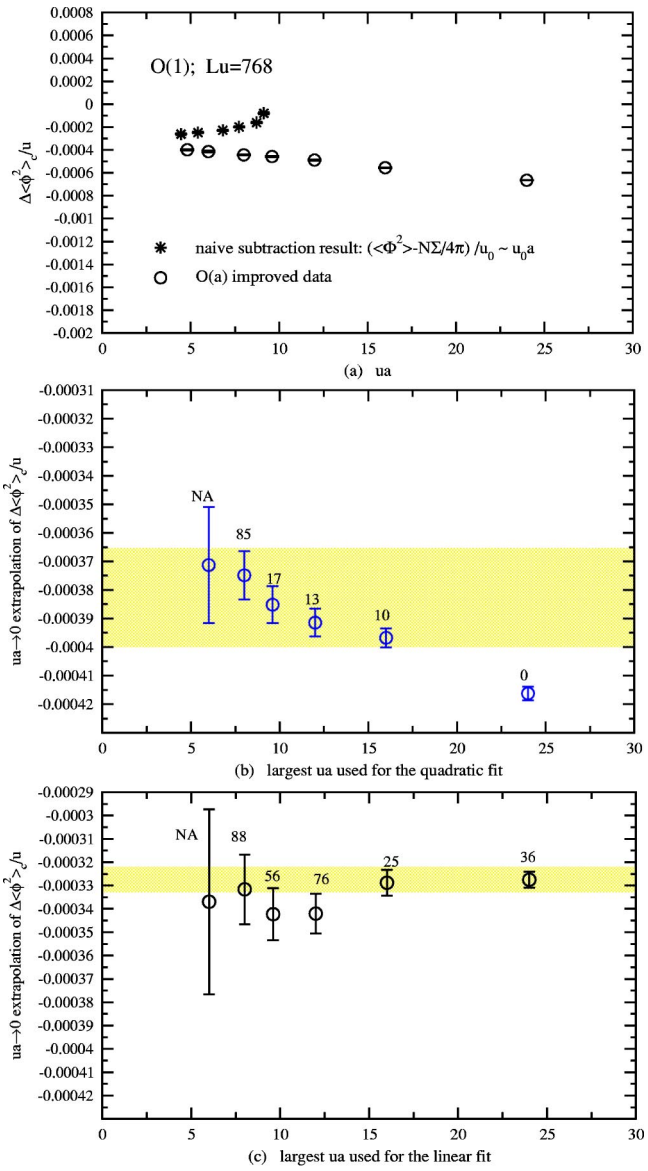

FIG. 2. Simulation results for $\Delta\langle\phi^2\rangle_c/u$ vs ua at fixed physical volume $(Lu)^*=768$ for O(1). The circular data are obtained from Eq. (2.5), with $\delta\phi^2$ being given by Eq. (2.6a). The star data are obtained using the naive lattice result $\Delta\langle\Phi^2\rangle_L\equiv(\langle\Phi^2\rangle-N\Sigma/4\pi)/u_0$. It has linear+linear×logarithmic+quadratic dependence on ua. (b) gives the fitting results for the quadratic fit and (c) gives the fitting results for the linear fit.

$$\bar{\phi}\equiv\frac{1}{V}\int d^3x\,\phi(x). \tag{2.11}$$

The nominal phase transition is defined as occurring when $C=C^*$, where C^* is a universal value that improves convergence to the infinite-volume limit. C^* depends on the shape and boundary conditions of the total lattice volume but not on the short distance structure. For cubic lattice volumes with periodic boundary conditions, $C^*\simeq1.603(1)$ for O(1) [16] and $C^*\simeq1.095(1)$ for O(4) [17]. I have checked that the errors on C^* are not significant for the purposes of this application. Therefore, I have used the central values for the nominal C^*.

TABLE II. Fitting results for $\Delta\langle\phi^2\rangle_c/u$ and r_c/u^2 using formula (2.15). In the case of $\Delta\langle\phi^2\rangle_c/u$, both a linear fit result and a quadratic fit result for B_1 are given. The final values are assigned to cover both fit results.

		$\Delta\langle\phi^2\rangle_c/u$						
		$A_1+A_2(Lu)^{-d+y_t}$ fit		$B_1+B_2(ua)^2$ fit	$B_1+B_2'(ua)$ fit	$\Delta\langle\phi^2\rangle_c/u=B_1-A_2\times(Lu)^{-d+y_t}$		
N	$(Lu,ua)^*$	A_1	$A_2\times(Lu)^{-d+y_t}$	B_1		$O(ua)^2$	$O(ua)$	Final
1	(768,12)	−0.0006199(40)	0.0001335(50)	−0.000383(17)	−0.003275(55)	−0.000517(18)	−0.0004610(74)	−0.000494(41)
4	(144,3)	−0.003023(92)	0.002978(92)	0.000007(26)	0.000163(37)	−0.002971(96)	−0.002815(99)	−0.00289(18)

		r_c/u^2			
		$C_1+C_2(Lu)^{-y_t-\omega}$ fit		$D_1+D_2(ua)$ fit	
N	$(Lu,ua)^*$	C_1	$C_2(Lu)^{-y_t-\omega}$	D_1	$r_c/u^2=D_1-C_2(Lu)^{-y_t-\omega}$
1	(768,12)	0.00274001(28)	−0.00000178(22)	0.0015231(48)	0.0015249(48)
4	(144,3)	0.0035035(62)	−0.000183(12)	0.002375(10)	0.002558(16)

In practice, it never happens that the simulation is done precisely at r where $C=C^*$. I instead simply simulate at some $r=r_{\rm sim}$ close to it. I then use canonical reweighting of the time series data to analyze r's near $r_{\rm sim}$ and determine r and $\Delta\langle\phi^2\rangle$ at $C=C^*$.

A renormalization group analysis of the scaling of finite-volume errors shows that, when the method of Binder cumulants is used, the values of $\Delta\langle\phi^2\rangle_c$ and r_c scale at large volumes as [5]

$$\frac{\Delta\langle\phi^2\rangle_c}{u}\simeq A_1+A_2(Lu)^{-d+y_t}, \tag{2.12a}$$

$$\frac{r_c}{u^2}\simeq C_1+C_2(Lu)^{-y_t-\omega}, \tag{2.12b}$$

for fixed ua. Here $d=3$ is the dimension of space, $y_t=1/\nu$, and ν and ω are the standard O(N) critical exponents associated with the correlation length and corrections to scaling, respectively. The values of the exponents that I have used are[4]

$$\begin{aligned}&\text{O(1):}\quad y_t=1.587(1),\\ &\qquad\omega=0.84(4),\\ &\text{O(4):}\quad y_t=1.329(2),\\ &\qquad\omega=0.79(4).\end{aligned} \tag{2.13}$$

[4]A nice review and summary of the critical exponents can be found in Ref. [12]. For the case of O(1), we have used their summarized values of $\nu=1/y_t$ and ω based on the calculation from high temperature (HT) expansion technique and Monte Carlo simulations. For comparison, some experimental results for y_t are 1.61(8) [13], 1.58(2) [14]. For O(4), Monte Carlo simulation for ν gives 0.7525(10) [15] (used by us), 0.749(2) [18]. From HT expansion: 0.759(3) [19]; from ϵ-expansion, 0.737(8) [20]. For ω, the only MC simulation result is $\omega=0.765$ (without quotation of error) from [18]. Reference [20] gives $\omega=0.774(20)$ ($d=3$ expansion) and 0.795(30) (ϵ-expansion). We have chosen the value to cover both of the errors for ω.

The large volume scaling of $\Delta\langle\phi^2\rangle_c/u$ depends only on y_t, which have errors $\sim$ 0.1% in both cases. They have a negligible effect on my final results. On the other hand, for the case of r_c/u^2, the large volume scaling depends on both y_t and ω. I will show that the errors of ω do have effects on the large volume errors of r_c/u^2. They are included in the final results.

For a discussion of higher-order terms in the large volume expansion, see Ref. [5], but the above will be adequate for this application. I will fit the large Lu data to the leading scaling forms (2.12) to extract the infinite-volume limit.

The basic procedure for extracting simultaneously the $ua\to 0$ and $Lu\to\infty$ limits of my result will be as follows.

(i) I first fix a reasonably small value of $(ua)^*$ of ua, take data for a variety of sizes Lu (to as large Lu as practical), and then extrapolate the size of finite-volume corrections, fitting the coefficients A_2 and C_2 of the scaling law (2.12).

(ii) Next, I instead fix a reasonably large physical size $(Lu)^*$ and take data for a variety of ua (to as small ua as practical), and extrapolate the continuum limit of our results at that $(Lu)^*$, which corresponds to fitting B_1 and D_1 of (2.8) and (2.9).

(iii) Finally, I apply to the continuum result of step (ii), the finite-volume correction for $(Lu)^*$ determined by step (i). In total, I have

$$\left\{\frac{\Delta\langle\phi^2\rangle_c}{u}\right\}_{final}=B_1-A_2((Lu)^*)^{-d+y_t}, \tag{2.14}$$

$$\left\{\frac{r_c}{u^2}\right\}_{final}=D_1-C_2((Lu)^*)^{-y_t-\omega}.$$

There is a finite lattice spacing error in the extraction of the large volume correction (i.e., A_2 and C_2). In Ref. [5], it is argued that this source of error is formally high order in $(ua)^*$ and so expected to be small.

III. SIMULATION RESULTS

A. O(1) results for $\Delta\langle\phi^2\rangle_c/u$

There is a practical tradeoff between how large one can take the system size $(Lu)^*$ in order to reach the large vol-

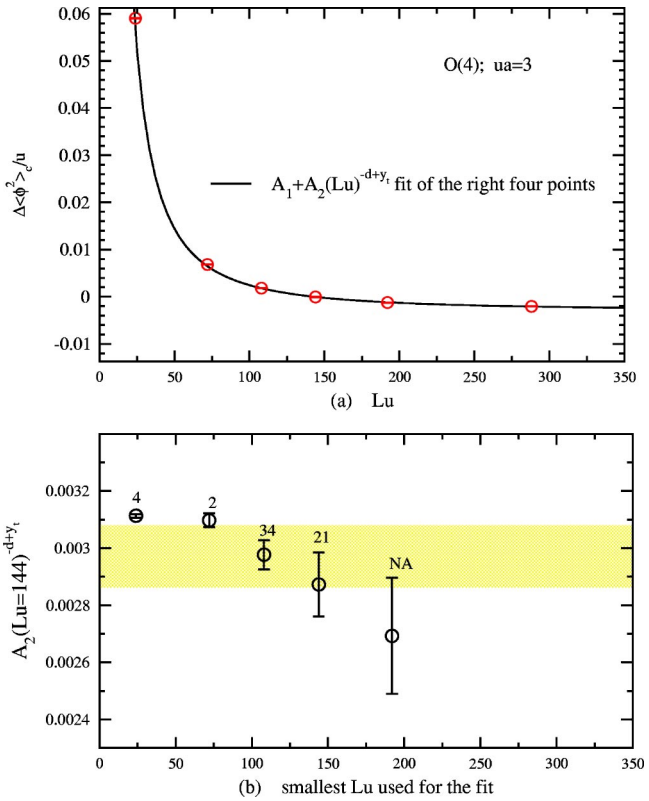

FIG. 3. As Fig. 1 but for O(4) at $ua=3$ with reference point $(Lu,ua)^*=(144,3)$.

ume limit versus how small one can take $(ua)^*$ in order to reach the continuum limit. Figure 1(a) and the lower points (circles) in 2(a) show, respectively, the Lu dependence at $(ua)^*=12$ and the ua dependence at $(Lu)^*=768$ for $\Delta\langle\phi^2\rangle_c/u$ in the O(1) model. From the Lu dependence, we can see that $(Lu)^*=768$ is a reasonably large value of Lu—the finite-volume corrections are moderately small. From the ua dependence, we can see that $(ua)^*=12$ is reasonably small.

Figure 1(b) shows the size $A_2(Lu)^{-d-y_t}$ at $(Lu)^*=768$ when fitting the Lu dependence of Fig. 1(a) to the scaling form (2.12a). The result of the fit, and its associated confidence level, depend on how many points are included in the fit. Percentage confidence levels are shown in the figure. My procedure will be to determine the best values of the fit parameters by including as many points as possible while maintaining a reasonable confidence level. Then to assign an error, I use the statistical error from including one less point in the fit. This will help avoiding the underestimation of systematic errors. The resulting estimate 0.000 133 5(50) of the finite-volume correction is depicted by the shaded bar in Fig. 1(b) and collected in Table II. The corresponding best fit is shown as the solid line in Fig. 1(a). Even though there is no direct use of it, I show for completeness the fit parameter A_1 in Fig. 1(c), which corresponds to the infinite-volume value of $\Delta\langle\phi^2\rangle_c/u$ at $(ua)^*=12$.

Having found the large volume extrapolated values, I will now move on to the $ua\to 0$ limit for $\Delta\langle\phi^2\rangle_c/u$ at a fixed physical volume $(Lu)^*=768$. Theoretically, from the argu-

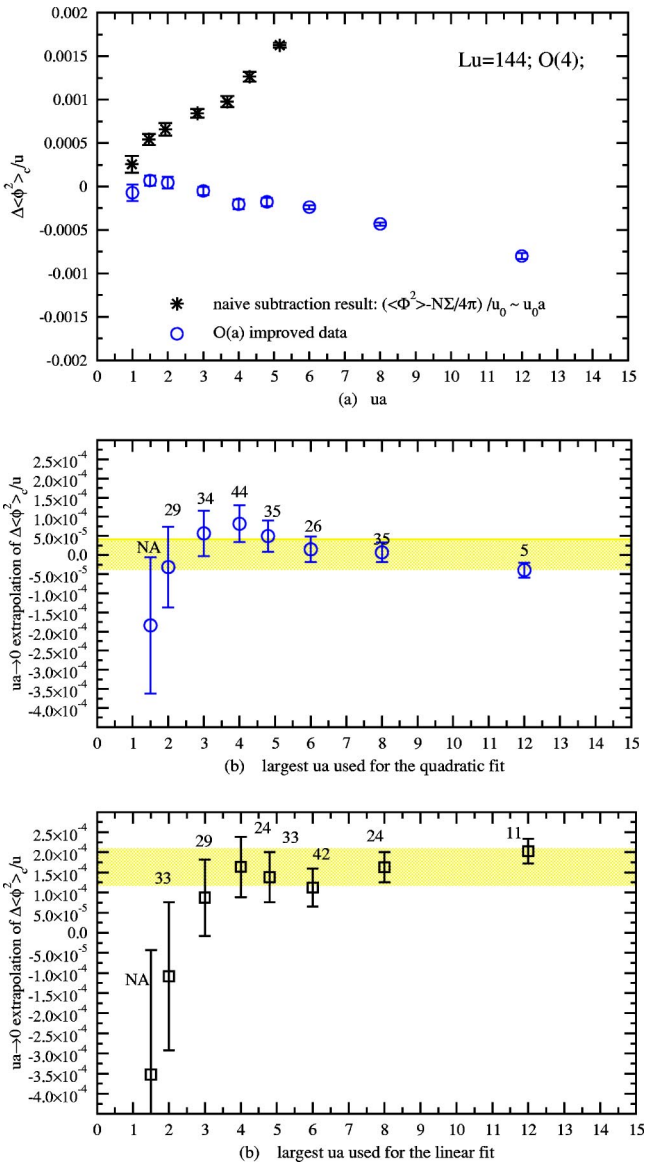

FIG. 4. As Fig. 2, but for O(4) at $(Lu)^*=144$. The triangular data in (a) is again the naive lattice result $\Delta\langle\Phi^2\rangle_L/u_0$ which shows again bigger lattice errors than the $O(a)$ improved data (circular data).

ment of Ref. [5], if one uses the $O(a)$ improved formula (2.5) to obtain the continuum approximated $\Delta\langle\phi^2\rangle_c/u$, the remaining lattice error should be $\sim O(ua)^2$.

The circular data in Fig. 2(a) show the $O(a)$ improved simulation results by using Eq. (2.5). First I have tried a quadratic fit with the form $B_1+B_2(ua)^2$. The fitting results for B_1 are given by Fig. 2(b). One can see while a three-point $(ua\leqslant 8)$ fit gives an impressive confidence limit (C.L.) of 85%, including the fourth point $(ua=9.6)$ reduces the CL to 17%. However, adding two more points keeps the CL above 10%. Due to this feature, it is hard to determine the last point that should be fit to the quadratic formula. Instead, I assigned the value to cover all the 85%, 17%, 13%, and 10% CLs which gives $-0.000\,383(17)$. The result is indicated by the shaded area.

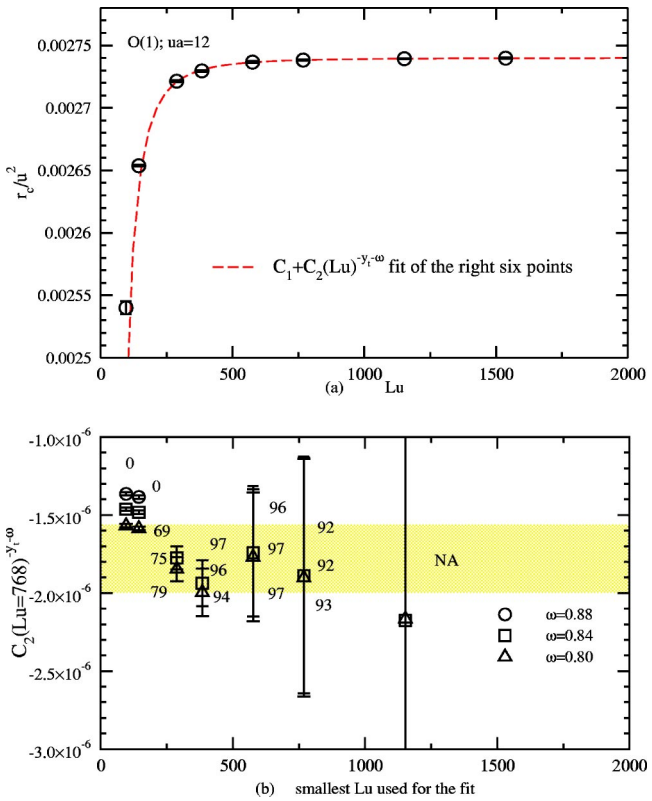

FIG. 5. Simulation results for r_c/u^2 vs physical volume for O(1) at $ua=12$ with $(Lu,ua)^*=(768,12)$. We have used three values for ω for the fits. The confidence levels for all the fits are listed in the same vertical order as the legend. The final assignment covers all the three extrapolations. The changes of the extrapolated $C_2(Lu)^{-y_t+\omega}$ is about one error bar due to the uncertainty in ω.

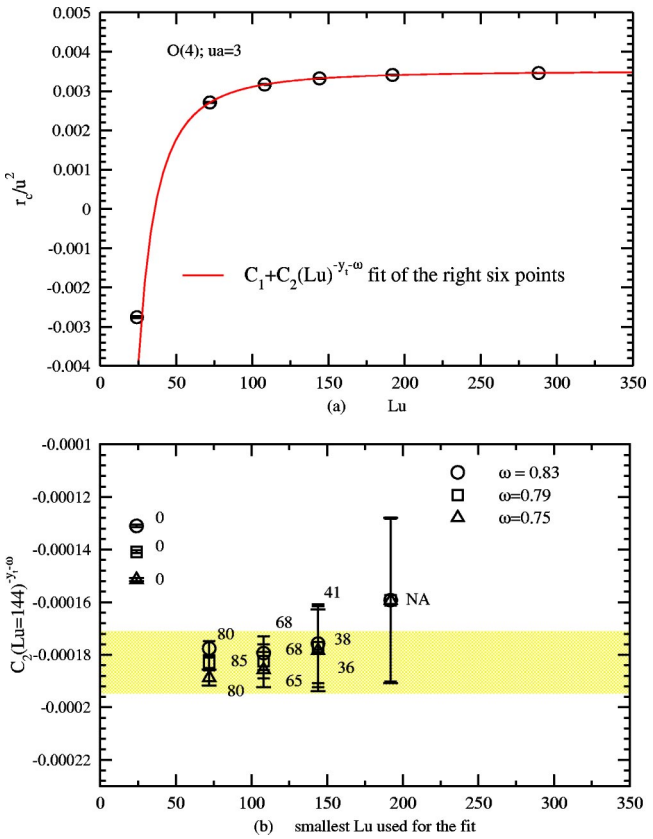

FIG. 6. As Fig. 5 but for O(4) at $ua=3$ with $(Lu,ua)^*=(144,3)$.

The poor behavior of the quadratic fit makes one wonder if the data is actually more ''linear'' than ''quadratic.'' To check this, I refit the circular data using a linear function (2.9a). The results are shown in Fig. 2(c). Surprisingly, I can fit all the data points with a very good CL. The $ua\to 0$ extrapolated value in this case is $-0.000\,3275(55)$, which is very different from the quadratic fit result. The obvious linear behavior of the data seem to indicate that there might be some residual $O(a)$ coefficient in Eq. (2.5) that has not been accounted for. Given this uncertainty, I have used both the linear and quadratic extrapolated results, combined with the error due to the finite lattice size to obtain two continuum values (Table II). They differ by about 10%, which is considered my systematic error. The final result is assigned to cover both results and is tabulated in Tables II and I.[5]

As a comparison, I have also shown the naive subtracted result given by $\Delta\langle\Phi^2\rangle_L/u_0\equiv(\langle\Phi^2\rangle-N\Sigma/4\pi)/u_0$ vs the unimproved u_0a as the scale based on the same simulation [the stars in Fig. 2(a)]. One can see that the finite lattice spacing errors is more explicit with the stars, corresponding to the unimproved data, than that of the circles, corresponding to the improved ones [using Eq. (2.5)]. Theoretically, $\Delta\langle\Phi^2\rangle_L/u_0$ data have logarithmic×linear and linear dependences on u_0a.

B. r_c and O(4) results

Figures 3 and 4 show similar curves for the O(4) model, where we have taken $(Lu)^*=144$ and $(ua)^*=3$ as a reasonably large size and reasonably small lattice spacing. It's worth noting that the large N limit predicts the distance scale that characterizes the physics of interest should scale as $1/(Nu)$. That leads one to expect that the upper limit for ''reasonably small'' values of ua and lower limit for ''reasonably large'' values of Lu should scale roughly as $1/N$.

The fitting proceeds as in the O(1) case. For the Lu-fixed data of $\Delta\langle\phi^2\rangle_c/u$ (Fig. 4), I have again fitted the data with both linear and quadratic functions. Both the quadratic fit and the linear fit can go up to $ua=8$ while keeping good CLs. However, their $ua\to 0$ extrapolations are also different (see Fig. 4 and Table II for the fitting results). The final continuum value is assigned to cover both extrapolations.

The analysis of the result for r_c/u^2 in both the O(1) and O(4) models is much the same (Figs. 5–7). For the large volume extrapolations, since the critical exponent ω has a larger uncertainty ($\sim 5\%$), I have used three different values

[5]In Ref. [5], for the case of O(2) model, the Lu fixed data are fitted by quadratic functions only. The $Lu=144$ data can be fitted also by a linear function. The $Lu=576$ data on the other hand can be fitted by only a quadratic function for the first four points. However, if one takes off the smallest ua point, the rest four points can be fitted very well by a straight line too. This might indicate that there could also be some linear coefficients in the O(2) theory. For more discussions on this possible linear coefficient, see Ref. [23].

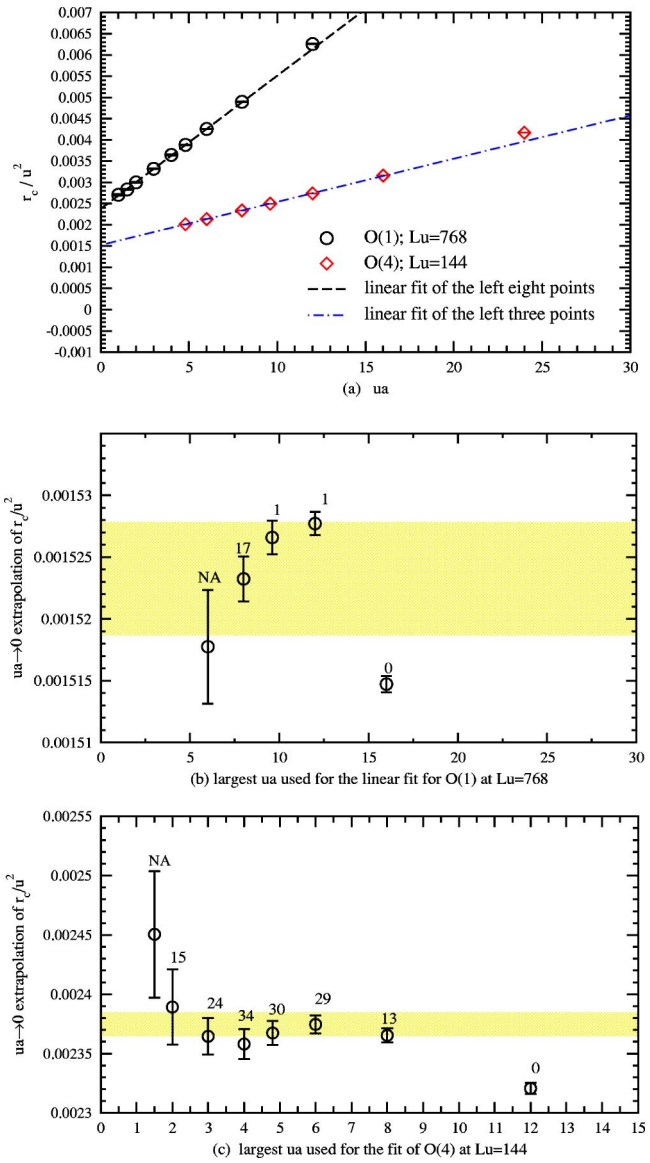

FIG. 7. Simulation results for r_c/u^2 vs ua for O(1) at $(Lu)^*=768$ and for O(4) at $(Lu)^*=144$. The two straight lines in (a) are linear fits to the data.

of ω (maximum, central, minimum) for both O(1) and O(4)'s cases. The final results of the $C_2(Lu)^{-y_t-\omega}$ value cover all the three different extrapolated values. This difference results in about 1% of the error quoted in the final results for r_c/u^2. For the Lu fixed data, since there is no improvement of $O(a)$ errors, the continuum extrapolation of the data taken at fixed Lu are fitted to linear behavior in ua, following Eq. (2.8b) or Eq. (2.9b). The fitting results are again summarized in Tables I and II.

IV. CONCLUSION

Figure 8 and Table II show a comparison of the simulation results for $\Delta\langle\phi^2\rangle_c/u$ with the NLO result (1.5) for $N=1,2,4$. The $N=1,4$ cases are from this paper. The result of

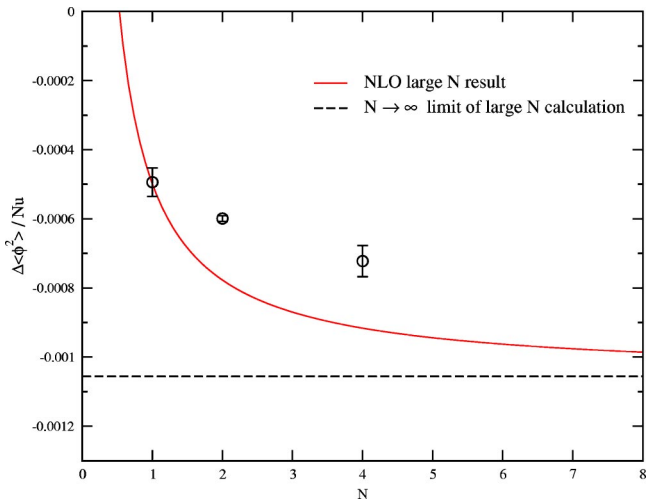

FIG. 8. Comparison of NLO large N result with simulation results for O(1), O(2), and O(4). The solid line is the NLO large N result for $\Delta\langle\phi^2\rangle_c/Nu$ and the dashed line is the $N=\infty$ value.

O(2) model is taken from Ref. [5].[6] In the figure, I have actually plotted $\Delta\langle\phi^2\rangle_c/(Nu)$, where the explicit factor of N factors out the leading-order dependence on N as $N\to\infty$. Amusingly, the large N estimate for $N=1$ seems to be the most accurate of the three cases. This is presumably an accident—the result of the large N approximation just happens to be crossing the set of actual values near $N=1$. From Eq. (1.5), the error for $\Delta\langle\phi^2\rangle_c/Nu$ should scale as $1/N^2$, but there is clearly no sign of such behavior between $N=2$ and $N=4$. This might indicate that $N=4$ is still too small for the error in the large N approximation to scale properly. It would be interesting to numerically study yet higher N such as $N=8$ or $N=16$ to attempt to verify the details of the approach to the large N limit.

For the systematic error due to the possible linear behavior in the $ua\to0$ extrapolation of $\Delta\langle\phi^2\rangle_c/u$, so far no theoretical reasoning is found. It would be interesting to reinvestigate the matching calculations given in Ref. [5].

ACKNOWLEDGMENTS

I would like to thank the Physics Department of the University of Virginia for providing me the opportunity and support for this research work. The work was supported, in part, by the U.S. Department of Energy under Grant No. DE-FG02-97ER41027. I am especially grateful to P. Arnold for his valuable guidance and assistance throughout the research work.

APPENDIX: TABULATED DATA

Tables III and IV are a collection of all the data reported in this paper. The standard integrated decorrelation time τ for a single operator O is defined as

[6]If one also considers the systematic uncertainty in the $ua\to0$ extrapolation in Ref. [5], then the result for O(2) should have a higher systematic uncertainty.

TABLE III. Collection of O(1) simulation data.

O(1)						
Lu	L/a	ua	r_c/u^2	$\Delta\langle\phi^2\rangle_c/u$	τ_{decorr}	$N_{\mathrm{sweeps}}/2\tau$
8	8	1	−0.01975(18)	0.14599(50)	0.8	61617
12	12	1	−0.00901(12)	0.07718(41)	0.9	58809
24	8	3	−0.001194(44)	0.02577(14)	1.1	47134
36	12	3	0.000437(31)	0.01332(11)	1.1	46288
48	16	3	0.001059(10)	0.008149(54)	1.1	44135
96	8	12	0.0025401(52)	0.002530(23)	2.5	20188
144	12	12	0.00265373(60)	0.0010371(26)	2.3	590789
192	32	6	0.0020919(35)	0.000446(20)	3.5	7175
288	24	12	0.00272132(81)	−0.0000604(44)	4.3	53716
384	32	12	0.00272961(71)	−0.0002622(36)	5.8	19281
576	48	12	0.00273662(70)	−0.0004271(50)	11.3	6731
768	128	6	0.00213384(75)	−0.0004142(63)	1.6*	4795
768	160	4.8	0.00201051(74)	−0.0003987(61)	2.8*	1643
768	32	24	0.00416985(16)	−0.0006645(23)	3.7	13690
768	48	16	0.00315905(45)	−0.0005548(39)	11.5	8800
768	64	12	0.00273822(48)	−0.0004886(51)	8.9	22219
768	80	9.6	0.00249587(61)	−0.0004567(42)	1.3*[7]	4545
768	96	8	0.00233612(56)	−0.0004429(39)	2.7*	15260
1152	96	12	0.00273936(42)	−0.0005441(33)	3.7*	3480
1536	128	12	0.00273977(41)	−0.0005679(33)	7.5*	1411

TABLE IV. Collection of O(4) simulation data.

O(4)						
Lu	L/a	ua	r_c/u^2	$\Delta\langle\phi^2\rangle_c/u$	τ_{decorr}	$N_{\mathrm{sweeps}}/2\tau$
4	4	1	−0.13588(100)	1.1014(54)	0.9	53759
8	4	2	−0.04051(27)	0.3673(17)	0.9	112355
12	4	3	−0.0182(17)	0.193(13)	0.5	100000
16	4	4	−0.00913(11)	0.11794(55)	1.6	60697
24	8	3	−0.002756(22)	0.05904(11)	1.1	465111
32	16	2	−0.000403(54)	0.03485(29)	1.0	25913
48	16	3	0.001792(22)	0.01641(13)	1.1	44839
72	24	3	0.002709(11)	0.006827(59)	1.4	58782
108	36	3	0.0031673(87)	0.001814(54)	1.9	26085
144	12	12	0.0062556(51)	−0.0008(34)	1.7	57244
144	144	1	0.002704(17)	−0.000072(95)	4.6	4416
144	18	8	0.0048967(29)	−0.000431(18)	2.3	154272
144	24	6	0.0042556(34)	−0.000238(22)	2.3	83972
144	30	4.8	0.0038808(76)	−0.000177(48)	2.8	18519
144	36	4	0.0036449(94)	−0.000204(57)	2.5	47481
144	48	3	0.003318(66)	−0.000051(47)	1.6	47051
144	72	2	0.002998(12)	0.000045(67)	3.3	8952
144	8	18	0.0087128(29)	−0.000018(41)	1.1	44435
144	9	16	0.0077983(67)	−0.000689(62)	1.0	452306
144	96	1.5	0.0028309(98)	0.000069(60)	3.2	11499
192	64	3	0.0034097(76)	−0.001234(46)	2.8	15893
288	96	3	0.0034596(63)	−0.002053(42)	7.7	5792

$$\tau \equiv \frac{1}{2} + \sum_{n=1}^{\infty} \frac{C(n)}{C(0)}, \tag{A1}$$

where

$$C(n) = \frac{1}{(N-n)} \sum_{i=1}^{N-n} A_i A_{i+n} - \left(\frac{1}{N} \sum_{i=1}^{N} A_i \right)^2 \tag{A2}$$

is the autocorrelation function associated with the operator A. In practice, the sum in Eq. (A1) is cut-off when $C(n)/C(0)$ first drops below 0.05 because of the statistical fluctuation in $C(n)$. The nominal decorrelation time listed in Tables III and IV[7] is the largest value of the various operators required in the computations of the Binder cumulant and $\Delta\langle\phi^2\rangle_c/u$ by using the canonical reweighting method (Ref. [5]).

[7]Numbers with * means the simulation data that are collected every $10\tau_{decorr}$ sweeps.

[1] G. Baym, J.-P. Blaizot, M. Holzmann, F. Laloë, and D. Vautherin, Phys. Rev. Lett. **83**, 1703 (1999).
[2] P. Arnold, G. Moore, and B. Tomášik, Phys. Rev. A **65**, 013606 (2002).
[3] M. Holzmann, G. Baym, J.P. Blaizot, and F. Laloë, Phys. Rev. Lett. **87**, 120403 (2001).
[4] V.A. Kashurnikov, N.V. Prokof'ev, and B.V. Svistunov, Phys. Rev. Lett. **87**, 120402 (2001); **87**, 160601 (2001).
[5] P. Arnold and G. Moore, Phys. Rev. E **64**, 066113 (2001).
[6] P. Arnold and G. Moore, Phys. Rev. Lett. **87**, 120401 (2001).
[7] F.F. de Souza Cruz, M.B. Pinto, R.O. Ramos, and P. Sena, Phys. Rev. A **65**, 053613 (2002); E. Braaten and E. Radesci, e-print cond-mat/0206186.
[8] G. Baym, J.-P. Blaizot, M. Holzmann, F. Laloë, and D. Vautherin, e-print cond-mat/0107129.
[9] G. Baym, J.-P. Blaizot, and J. Zinn-Justin, Europhys. Lett. **49**, 150 (2000).
[10] P. Arnold and B. Tomášik, Phys. Rev. A **62**, 063604 (2000).
[11] P. Arnold and B. Tomášik, Phys. Rev. A **64**, 053609 (2000).
[12] A. Pelissetto and E. Vicari, e-print cond-mat/0012164.
[13] D.M. Sullivan, G.W. Neilson, H.E. Fisher, and A.R. Rennie, J. Phys.: Condens. Matter **12**, 3531 (2000).
[14] B.H. Chen, B. Payandeh, and M. Robert, Phys. Rev. E **62**, 2369 (2000); **64**, 042401 (2001).
[15] H.G. Ballesteros, L.A. Fernández, V. Martin-Mayor, and A. Muñoz Sudupe, Phys. Lett. B **387**, 125 (1996).
[16] H. Blöte, E. Luijten, and J. Heringa, J. Phys. A **28**, 6289 (1995); H.G. Ballesteros *et al.*, *ibid.* **32**, 1 (1999).
[17] M. Hasenbusch, J. Phys. A **34**, 8224 (2000).
[18] M. Hasenbusch, Int. J. Mod. Phys. C **12**, 911 (2001).
[19] P. Butera and M. Comi, Phys. Rev. B **56**, 8212 (1997).
[20] R. Guida and J. Zinn-Justin, J. Phys. A **31**, 8103 (1998).
[21] J. Goodman and A.D. Sokal, Phys. Rev. D **40**, 2035 (1989).
[22] K. Binder, Phys. Rev. Lett. **47**, 693 (1981); Z. Phys. B: Condens. Matter **43**, 119 (1981).
[23] X. Sun, Ph.D thesis, University of Virginia, 2002.