Atomic Quantum Simulation of the Lattice Gauge-Higgs Model: Higgs Couplings and Emergence of Exact Local Gauge Symmetry

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Recently, the possibility of quantum simulation of dynamical gauge fields was pointed out by using a system of cold atoms trapped on each link in an optical lattice. However, to implement exact local gauge invariance, fine-tuning the interaction parameters among atoms is necessary. In the present Letter, we study the effect of violation of the U(1) local gauge invariance by relaxing the fine-tuning of the parameters and showing that a wide variety of cold atoms is still to be a faithful quantum simulator for a U(1) gauge-Higgs model containing a Higgs field sitting on sites. The clarification of the dynamics of this gauge-Higgs model sheds some light upon various unsolved problems including the inflation process of the early Universe. We study the phase structure of this model by Monte Carlo simulation, and also discuss the atomic characteristics of the Higgs phase in each simulator.

In addition, we find that the cold atoms in question may be used as a quantum simulator of a wide class of U(1) gauge-Higgs model, i.e., a Ginzburg-Landau-type model in the London limit coupled with the gauge field, the dynamics of which should offer us important insights on several fields including inflational cosmology\textsuperscript{11}.

Let us start with the path-integral representation of the partition function $Z$ of the compact U(1) pure LGT, the reference system of the present study:

$$Z = \int [dU] \exp(A), \quad A = \sum_{x,\mu} U_x^\dagger U_{x+\mu} + c.c.,$$

$$U_{x+\mu} = \exp(i\theta_{x+\mu}), \quad \theta_{x+\mu} = \nabla_x \theta_{x+\mu} - \nabla_{\mu} \theta_x,$$

where $x = (x_1, x_2, x_3, x_4)$ is the site index of the 3+1=4D lattice ($x_4$ is the imaginary time in the path-integral approach) and $\mu$ and $\nu$ ($= 1, 2, 3, 4$) are the direction indices that we also use as the unit vectors in the $\mu$ and $\nu$-th directions. The angle variable $\theta_{x+\mu} \in [0, 2\pi)$ and its exponential $U_{x+\mu}$ are the gauge variables defined on the link $(x, x+\mu)$. The bar in $\bar{U}_{x+\mu}$ implies complex conjugate, and $c_2(\equiv 1/\epsilon^2)$ is the inverse self-gauge-coupling constant. The product of four $U_{x+\mu}$ is invariant under the local (x-dependent) U(1) gauge transformation,

$$U_{x+\mu} \rightarrow U_{x+\mu}' = V_{x+\mu} U_{x+\mu} V_{x+\mu}^\dagger, \quad V_x = \exp(i\Lambda_x),$$

and so are the field strength $\theta_{x+\mu}$ and the action $A$. It is known\textsuperscript{17} that the system has a weak first-order phase transition at $c_2 = c_{2c} \simeq 1.0$. For $c_2 < c_{2c}$ ($> c_{2c}$) the system is in the confinement (Coulomb) phase in which the fluctuations of $\theta_{x+\mu}$ are strong (weak). In the Coulomb phase, $\theta_{x+\mu}$ describes almost-free massless particles, which correspond to photons in electromagnetism\textsuperscript{16}.
To obtain the quantum Hamiltonian $\hat{H}$ for $Z$, let us focus on the space-time plaquette term $\cos \theta(\tau, x)$ in $Z$ with the spatial direction index $i(=1, 2, 3)$ and rewrite it as

$$\exp \left( c_2 \cos \theta(\tau, x) \right) \simeq \sum_{m_v \in \mathbb{Z}} \exp \left[ -\frac{c_2}{2} (\theta(\tau, x) - 2\pi m_v)^2 \right]$$

$$\propto \sum_{E_{\tau} \in \mathbb{Z}} \exp \left[ -i E_{\tau} (\nabla \theta(\tau, x) - \nabla_4 \theta(\tau, x)) - \frac{1}{2 c_2} E_{\tau}^2 \right], \quad (3)$$

where we used the Villain (periodic Gaussian) approximation in the first line and Poisson’s summation formula in the second line. The term $i E_{\tau} (\nabla \theta(\tau, x) - \nabla_4 \theta(\tau, x))$ is the imaginary time and $\dot{f} \equiv df/d\tau$ shows that the integer-valued field $E_{\tau}$ on the spatial link $(x, x + i)$ is the conjugate momentum of $\theta(\tau, x)$. The corresponding operators at spatial site $r = (x_1, x_2, x_3)$ satisfy the canonical commutation relation $[\hat{E}_{\tau}, \hat{\theta}_{\tau, r}] = -i \delta_{\tau, \tau'} \delta_{r, r'}$.

The operator $\hat{E}_{\tau}$ represents the electric field in electromagnetism but has integer eigenvalues owing to the compactness (periodicity) of $A$ under $\theta_{\tau, x} \rightarrow \theta_{\tau, x} + 2\pi$. The integration over $\theta_{\tau, x}$ can be performed as

$$\hat{G} \equiv \int \prod_i d\theta_{\tau, x} \exp(-i \sum_{x, i} E_{\tau} \nabla \theta_{\tau, x}) = \prod_x \delta Q_{x=0, r}, \quad (4)$$

where we used $\sum_{x, i} E_{\tau} \nabla \theta_{\tau, x} = -\sum_{x, i} \nabla_i E_{\tau} \theta_{\tau, x}$, which holds for a lattice with periodic boundary conditions.

One may check that the quantum Hamiltonian $\hat{H}$ which gives $Z$ at the inverse temperature $\beta$ is just the one given by Kogut and Susskind [15],

$$\hat{H} = \frac{1}{2 c_2 \Delta \tau} \sum_{r,i} E_{\tau}^2 - \frac{c_2}{\Delta \tau} \sum_{r < i, j} \cos \theta_{r, ij} \quad (5)$$

with $\Delta\tau \equiv \beta/N$ being the short-time interval in the $\tau$ direction. The $\cos \theta_{r, ij}$ term corresponds to the magnetic energy $(\nabla \times \mathbf{A})^2$ in the continuum [16]. In fact, by inserting the complete sets $1_{\hat{G}} = \prod_{\tau} \prod_{x} E_{\tau}, |\{E_{\tau}\}|/|\{E_{\tau}\}|$ and $1_{\theta} = \prod_{\tau, r} \int d\theta_{\tau, r} |\{\theta_{\tau, r}\}|/|\{\theta_{\tau, r}\}|$ in between the short-time Boltzmann factors $\exp(-\Delta\tau \hat{H})$, one may derive the relations $Z = \text{Tr} \hat{G} \exp(-\hat{H}), \quad \hat{G} \equiv \prod_\tau \delta_{Q_{x=0, r}}, \quad$ and $\hat{Q}_r \equiv \sum_i \nabla_i \hat{E}_{\tau} \quad [17]$. Here, $\hat{Q}_r$ is the generator of the time-independent gauge transformation and $\hat{H}$ respects this symmetry as $[\hat{H}, \hat{Q}_r] = 0$. The Gauss’ law $\hat{Q}_r = 0$ is to be imposed as a constraint for physical states.

Let us discuss the cold-atom studies [3] specifically focusing on the quantum simulator using Bose-Einstein condensation (BEC) in an OL [6]. We write the boson operator on the link as $\psi_{\tau, x} = \sqrt{\rho_0} \exp\left[-\frac{1}{2} \sum_{i} \theta_{\tau, i} \right], \quad (\dot{\theta}_{\tau, i} = (-\nabla_\tau \psi_{\tau, x})$, where we use the same letter $\theta_{\tau, i}$ as $\theta_{\tau, x}$ in Eq. (1) because the former is to be identified as the latter. We start with the following atomic Hamiltonian [6],

$$\hat{H}_a = \sum_{r, a, b} \left\{ g_{ab} \rho_{\tau, r} \rho_{\tau, r'} + \frac{V_0}{2} \rho_{\tau, r}^2 + g_{ab} \psi_{\tau, r} \psi_{\tau, r'} + \text{H.c.} \right\}, \quad (6)$$

where $a, b = 1 \sim 6$ counts the links emanating from each site. The $g_{ab}$-term describes the density-density interaction, the $V_0(>0)$-term is the on-link repulsion, and the $g_{ab}^2$-term is the hopping term induced by external electromagnetic fields. We assume that the average $\langle \rho_\tau \rangle = \rho_0$ is homogeneous and large, $\rho_0 \gg 1$, and set $\rho_{\tau, r} = \rho_0 + (-)^r \hat{\eta}_{\tau, r}$, where $\hat{\eta}_{\tau, r}$ is the density fluctuation. Then, by choosing $g_{ab}$ and $g_{ab}^2$ suitably as $g_{ab} = (g > 0)$ for any $a$ and $b$, $g_{ab}^2 \approx 0$ for parallel link pairs, $\hat{H}_a$ is rewritten effectively as

$$\hat{H}_a = \frac{1}{2g^2} \sum_r \left( \sum_{i} \nabla_i \hat{\eta}_{\tau, r} \right)^2 + V_0 \sum_{i} \hat{\eta}_{\tau, i}^2 + \hat{H}_L((\hat{\theta}_{\tau, r})),$$

$$\hat{H}_L = 2g' \rho_0 \sum_{r, i < j} \left( \cos(\theta_{\tau, r} - \theta_{\tau, j}) + \cdots \right), \quad (7)$$

The term with $\gamma^2 \equiv g^{-1}$ comes from the $g_{ab}$-term and represents the strength of the fluctuations $\eta_{\tau, r}$ around each site (partial conservation of atomic number). We note that setting $g_{ab}$ independent of $a, b$ and controlling its magnitude $\gamma = g^{-2}$ may be achieved by designing the OL suitably or by using interspecies Feshbach resonances [6,11]. Some theoretical ideas for the latter are also proposed [20]. $\hat{H}_L$ describes the phase correlation between the L-shaped nearest-neighbor (NN) links [the omitted terms in the sum are explicitly written in $A_L$ of Eq. (10) below]. We use the coherent state $|\{\psi_{\tau, r}\}\rangle$ and $1 = \prod_{r, i} \int d\rho_{\tau, r} |\{\psi_{\tau, r}\}\rangle \langle\{\psi_{\tau, r}\}|$ to obtain the path-integral for $Z_a = \text{Tr} \exp(-\beta \hat{H}_a)$ as

$$Z_a = \int \prod_r [d\eta_{\tau, r} d\theta_{\tau, r}] \exp \left[ \sum_{x, i} \left( -i \eta_{\tau, i} \nabla_4 \theta_{\tau, i} - \Delta \tau V_0 \eta_{\tau, i}^2 \right) - \frac{\Delta \tau}{2g^2} \sum_x \left( \sum_{i} \nabla_\tau \hat{\eta}_{\tau, i} \right)^2 - \Delta \tau \sum_x \hat{H}_L((\theta_{\tau, i})) \right]. \quad (8)$$

The first term in the exponent in R.H.S. comes from $\sum_{x, i} \psi_{\tau, x} \nabla_\tau \psi_{\tau, x} \approx i \sum_{x, i} \eta_{\tau, i} \nabla_4 \theta_{\tau, i}$ and shows that $-\hat{\eta}_{\tau, r}$ is the conjugate momentum of $\theta_{\tau, r}$, whereby $\hat{E}_{\tau} = -\hat{\eta}_{\tau}$. The Gaussian factor $G \equiv \prod_x \exp(-\Delta \tau/2g^2) Q_x^2$ in Eq. (6) with $Q_x \equiv -\sum_i \nabla_i \eta_{\tau, x}$ shows that the Gauss’ law $Q_x = 0$ of Eq. (11) is achieved by $G \propto \prod_x \delta(Q_x)$ only at $\gamma \rightarrow 0$, and it is now shifted for $\gamma > 0$ to a Gaussian distribution with $Q_x^2 \lesssim \gamma^2/\Delta \tau$. Thus, $\gamma$ is a parameter used to measure the violation of Gauss’ law. Note that $G$ may be written as

$$G \simeq \int_0^{2\pi} \prod_x \frac{d\theta_{\tau, r}}{2\pi} \exp \left( \frac{\gamma^2}{\Delta \tau} \cos \theta_{\tau, x} - i \theta_{\tau, x} \sum_i \nabla_\tau \eta_{\tau, x} \right). \quad (9)$$

By integrating Eq. (8) with Eq. (9) over $\eta_{\tau, x} \in (-\infty, \infty)$, one obtains a term $-\left(4\Delta \tau V_0\right)^{-1} \sum_i \nabla_\tau \eta_{\tau, x} \nabla_\tau \theta_{\tau, x}^2$, which is a part of Gaussian Maxwell term. However, this result should be improved to respect the periodicity under $\theta_{\tau, x} \rightarrow \theta_{\tau, x} + 2\pi$, because $\theta_{\tau, x}$ is the phase of the condensate. This Gaussian term is to be replaced, e.g., by a periodic Gaussian form or by the corresponding cosine
form cos $\theta_{x14}$ as in Eq. (8) (which may be achieved by summing over the integer $\eta_x$). After the summation over $\eta_x$, $Z_a$ may be expressed by the following general form:

$$Z_a = \int [dA] \exp(A_a), \quad A_a = A_1 + A_P + A_L,$$

$$A_1 = \sum_{x,\mu} c_1 \mu \cos \theta_{x\mu}, \quad A_P = \sum_{x,\mu<\nu} c_2 \mu \nu \cos \theta_{x\mu\nu},$$

$$A_L = \sum_{x,\mu<\nu} \left[ \cos(\theta_{x\mu} - \theta_{x\nu}) + \cos(\theta_{x\mu} + \theta_{x+\mu\nu}) \right],$$

$$\gamma \equiv \frac{3}{2} \gamma_2 \gamma_3$$

The anisotropic parameters in $A_a$ are given as follows: $c_{14} = \gamma^2/\Delta \tau, c_{1i} = 0$ and $c_{2ij} \approx (2\Delta \tau \nu_0)^{-1} H_L$. Here, for general values of $g'$ directly gives rise to the $A_1$ term with $c_{3i} = 0$ and $c_{3ij} = 2g' \nu_0 \Delta \tau$, while $c_{2ij} = 0$ [21]. We note that, for $g'$ much smaller than $\gamma^2$ and/or $\nu_0$, one may treat $H_L$ as a perturbation. In Refs. [3, 7, 10], the case $\gamma \approx 0$ is considered to enforce the Gauss’s law, and the second-order perturbation theory is invoked to obtain an anisotropic version of the Kogut-Susskind Hamiltonian [3] as an effective Hamiltonian for the gauge-invariant subspace. This implies $c_{2ij} \approx \gamma^2 r_0^2 \gamma^2 \Delta \tau$ and $c_{3ij} = 0$ in Eq. (10). We refer to this case later as the $\gamma \approx 0$ case.

Concerning to $c_{1i}$, we note that nonvanishing $c_{1i}$ terms may be incorporated into the cold-atom system by an idea discussed in Ref. [22]: one may couple to $\tilde{\psi}_r$ the atomic field $\tilde{a}_r$ in another hyperfine state held in a different trapping potential via the interaction $H_{a\psi} = \kappa \sum_r \tilde{a}_r^{\dagger} \tilde{\psi}_r + H.c$. If $\tilde{a}_r$ condenses uniformly at sufficiently high temperatures, $\tilde{a}_r$ works as a BEC reservoir and $H_{a\psi}$ supplies the $c_{1i}$ term effectively with $c_{1i} = 2\kappa |\langle a_r \rangle| \sqrt{\nu_0} \Delta \tau$. A similar idea is also discussed in Ref. [3] to generate the $c_{2ij}$ (spatial plaquette) term.

The $A_1$ and $A_L$ terms in Eq. (10) apparently break U(1) gauge invariance. However, the model $Z_a$ of Eq. (10) with general set of parameters is equivalent to another HGT with exact U(1) gauge invariance, i.e., the U(1) gauge-Higgs model containing a Higgs field $\phi_x$. The Higgs field is a complex field defined on site $x$ and takes the form $\phi_x = \exp(\phi_{x14})$, that is its radial excitation is frozen (so-called London limit). The partition function of the U(1) gauge-Higgs model $Z_{GH}(=Z_a)$ is defined by

$$Z_{GH} = \int [d\phi] [dU] \exp(A_GH(\{U_{xp}\}, \{\phi_x\}),$$

$$A_GH = A'_1 + A_P + A'_L, \quad \frac{dA_GH}{dU} = \prod_x \int_0^{2\pi} \frac{d\phi_{x14}}{2\pi},$$

$$A'_1 = \sum_{x,\mu} c_1 \mu \cos(\phi_{x\mu} + \theta_{x\mu} - \phi_{x+\mu}),$$

$$A'_L = \sum_{x,\mu<\nu} c_3 \mu \nu \left[ \cos(\phi_{x+\nu} + \theta_{x\mu} - \phi_{x\nu}) + \cos(\phi_{x+\nu} + \theta_{x\mu} + \theta_{x+\mu\nu} - \phi_{x\nu}) + \cos(\phi_{x+\nu} + \theta_{x+\mu\nu} - \phi_{x+\mu\nu}) \right].$$
FIG. 1. (Color online) Phase diagrams of the four models [14] in the $c_2-c_{1,3}$ plane determined by $U = \langle A \rangle$ and $C = \langle A^2 \rangle - \langle A \rangle^2$ calculated by MC simulations for a lattice size of $16^4$ [28]. The vertical axis is $c_1$ for Model IP, $c_3$ for Model PL, and $c_1 = c_3$ for Models ItPtLs and ItPLs. The confinement-Coulomb transition is missing in Model ItPtLs. The number (1, 2) at each critical point indicates its order of transition. The confinement-Higgs line of Model IP terminates at $c_2 \sim 0.8$.

only up to the phase boundary $c_{1(3)} = c_{1(3)}(c_2)$ (except for $c_2 \lesssim 0.8$ in Model IP); beyond this value of $c_{1(3)}$ the system enters into a new phase, the Higgs phase, in which both $\theta_{xy}^\mu$ and $\varphi_{x}$ are stable. The expectation that the cold atoms may simulate the pure gauge theory \[ R \[ 7 \[ 10 \] \] \] is assured qualitatively and generally as long as both systems are in the same phase. This occurs for the atomic parameters satisfying $c_{1(3)} < c_{1(3)}(c_2)$.

The confinement-Coulomb transition exists only for Models having $c_{2ij} \neq 0$ and $c_{2ij} \neq 0$; Model ItPtLs ($c_{2ij} = 0$) has no Coulomb phase. This is consistent with the results of pure U(1) gauge theory that the confinement-Coulomb transition exists for 4D system [17] but not in the 3D system [29]. For sufficiently large $c_{2ij}$ and $c_{2ij}$, $\theta_{xy}$ is almost frozen $\theta_{xy} \sim 0$ up to gauge transformation and the system reduces to the XY model with the XY spin $\varphi_{x} = \exp(\mathrm{i}\varphi_{x})$. Then, the $c_{1\mu}$ term becomes the NN spin-interaction, $c_{1\mu}\bar{\phi}_{x}\bar{\phi}_{x}$, and the $c_{3\mu
u}$ term becomes the next-NN one, $c_{3\mu
u}\bar{\phi}_{x}\bar{\phi}_{x}$. These (extended) XY models exhibit a second-order transition both for 3D and 4D couplings, which corresponds to the Higgs-Coulomb transition in Fig. 1. For small $c_{2\mu
u}$, the confinement-Higgs transition is missing in Model IP ($0 \leq c_2 \lesssim 0.8$), reflecting that $\theta_{xy}$ are decoupled at $c_2 = 0$ [29]. In contrast, in the other three Models, the $c_2$ term survives, couples another set of XY spins $\exp(\mathrm{i}\varphi_{x})$ on NN links, and gives rise to second-order transitions of the XY-model type at $c_2 \sim 0$.

It is quite instructive to clarify the physical meaning of the Higgs phase of the gauge system realized in atomic quantum simulators. In the simulator using bosons [6], the Higgs phase of the effective gauge system is nothing but the BEC state as the phase of the bosons (i.e., the gauge boson) is stabilized coherently. Therefore, the Higgs-confinement transition corresponds to the BEC transition. On the other hand, in Refs. [6, 11], the gauge field is expressed as $\tilde{U}_{r_1} \simeq (\xi_{r_1}^\dagger \xi_{r_2}^\dagger)^{1/2}$, and the Higgs phase corresponds to the state in which the quantum state at each link $(r, r + i)$ is given by a coherent superposition of the particle-number states such as $\vert 0 \rangle_{r, r + i} \langle 1 \vert_{r, r + i}$. In the double-well potential, this state is realized naturally, after which the Higgs phase of the gauge system appears easily.

This way of introducing U(1) variables [6, 11] reminds us of an approach starting with an antiferromagnet with $s = 1/2$ quantum spin at each site and obtaining the CP$^1$ + U(1) LGT [30], which has a Schwinger-boson (CP$^1$) variable at each site describing spins and an auxiliary but dynamical U(1) gauge variables on each link. Although the CP$^1$ + U(1) model and the present U(1) Higgs model are different from each other, their global phase structures are significantly similar (See Fig. 1 of Ref. [30]).

In summary, Eq. (11) is the target LGT of cold-atom systems that are basically those studied in Refs. [6, 7] but with more general values of interaction parameters and a possible atomic reservoir [6, 22]. Figure 1 predicts its global phase structures. From the discussion given in Refs. [6, 7, 22] and the relation (13), it may be rather universal that many cold-atom systems with multiplet (“quantum spins”) placed on OL links have their U(1) Higgs LGT counterparts. Such an equivalence between cold atoms and the U(1) gauge-Higgs model may be referred to as “quantum spin-gauge Higgs correspondence”.

FIG. 2. (Color online) Contour plot of the deviation of typical atomic density $\Delta \rho_r \equiv \sum_i \eta_i^2 / 3^{1/2}$ in the $x_1 - x_2$ plane at $x_3 = 0$ with external sources of atoms $\Delta \rho_{ext} = \pm \rho_1$ placed on the links emanating from $r = r_\pm = (\pm 0.4, 0, 0)$. The white regions have $\Delta \rho_r$ greater than a certain value and the darker regions have lower $\Delta \rho_r$. The atomic density on the link $(r, r + i)$ is given by $\rho_{i,j} = \rho_0 + \eta_i$, (here we discard the factor $-\) in front of $\eta_i$ for simplicity), and the deviation $\eta_i$ is calculated by using the electric field $E_{i,j} = -\eta_i$ with a pair of external sources $q = \pm 1$ at $r = r_\pm$. In the Higgs phase, $\Delta \rho_r$ decreases rapidly away from the sources. In the confinement phase, the deviation propagates from one source to the other along a one-dimensional string (electric flux).
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Atomic Quantum Simulation of Lattice Gauge-Higgs Model: Higgs Couplings and emergence of exact gauge symmetry—Supplemental Material—

In this supplemental material, we explain some details to obtain the phase diagram Fig. 1, in particular, how to locate the transition points and determine the order of those transitions. For this purpose, we measure the internal energy \( U = \langle A \rangle \) and the specific heat \( C = \langle A^2 \rangle - \langle A \rangle^2 \) by MC simulations \([1]\). We use the standard Metropolis algorithm \([2]\) with the periodic boundary condition for the lattice of size \( V = L^4 \) with \( L \) up to 24. The typical number of sweeps is 30000 + 3000 \( \sim \) 100000 + 10000 \( \ast \) 10, where the first number is for thermalization and the second number is for measurement. The errors of \( U \) and \( C \) are estimated by the standard deviation over 10 samples. Acceptance ratios in updating variables are controlled to be 0.6 \( \sim \) 0.8. We check that the hot start (\( \theta_{x\mu}, \phi_{x\mu} \) are chosen randomly between \([0, 2\pi]\)) and the cold start (\( \theta_{x\mu} = \phi_{x\mu} = 0 \)) give the same results within error margin. The results of \( U \) and \( C \) are checked also by (i) comparison with the high-temperature expansion up to \( O(c_1^4) \), which is valid for small \( c_1 \), and (ii) comparison at large \( c_2 \) with independent simulations with setting \( U_{x\mu} = 1 \) which should give similar transition point. In addition, for Model IP in Eq. (14), we make (iii) comparison with the analytic result at \( c_2 = 0 \) (see Ref. [23] in the text) and (iv) comparison with the result by Jansen et al. \([3]\) in which they study the phase structure of a similar model (Model IP with the radial component of Higgs field \( \phi_x \) being included).

Let us pick up some typical transition points for the Model IP in Eq. (14). Every curve of \( U \) and \( C \) shown below is obtained by first increasing the parameter \( c_1 \) or \( c_2 \) in a fixed interval with an increment \( \Delta c_1(2) \) and then decreasing it. Such a go-and-back run is useful to detect a hysteresis effect. According to their definitions in thermodynamics, a first-order transition has (i) a gap or a hysteresis loop in \( U \) and (ii) a sharp peak in \( C \) which usually develops in proportional to the system size \( V \), while a second-order transition has (i) a continuous \( U \) and (ii) a gap in \( C \). In many cases of second-order transitions, \( C \) shows a peak which connects lower and higher-valued regions of \( C \) and the peak hight develops as the system size is increased \([4]\).

In Fig. 3 we show \( U \) and \( C \) vs. \( c_1 \) for \( c_2 = 2.5 \). The curve \( U \) itself as a function of \( c_1 \) is almost continuous except for a small hysteresis loop at \( c_1 \sim 0.315 \), but its derivative with respect to \( c_1 \) seems to have a change (almost a gap) at \( c_1 \sim 0.315 \). Correspondingly, the curve \( C \) globally changes its value from the lower one around \( \sim 2.2 \) to the higher one around \( \sim 4.0 \) in the short interval \( 0.313 \lesssim c_1 \lesssim 0.319 \). These two behaviors accord with the definition of a second-order transition and therefore we conclude that a second-order transition takes place at \( 0.313 \lesssim c_1 \lesssim 0.319 \). Absence of no sharp peak indicates that the associated critical exponent \( \sigma \) is small \([4]\). We judge the hysteresis loop in \( U \) is too small as an evidence for a first-order transition.

![FIG. 3. (Color online) \( U/V \) and \( C/V \) vs. \( c_1 \) for \( c_2 = 2.5 \) \((L = 16)\). They indicate a second-order transition at \( 0.314 \lesssim c_1 \lesssim 0.322 \).](image)

In Fig. 4 we show \( U \) and \( C \) as a function of \( c_1 \) for \( c_2 = 0.9 \). The clear hysteresis loop indicates the existence of a first-order transition at \( 0.468 \lesssim c_1 \lesssim 0.478 \). The size

![FIG. 4. (Color online) \( U/V \) and \( C/V \) vs. \( c_1 \) for \( c_2 = 0.9 \) \((L = 16)\). A first-order transition takes place at \( 0.468 \lesssim c_1 \lesssim 0.478 \).](image)
of corresponding peaks in $C$ seems not large enough as a first-order transition, but such a phenomenon often takes place and is attributed to the finiteness of $\Delta c_1$.

In Fig. 5 we show $U$ as a function of $c_1$ for $c_2 = 0.85$ (top) and $c_2 = 0.80$ (bottom). For $c_2 = 0.85$, $U$ exhibits a step-function-like behavior at $c_1 \simeq 0.524$, although no hysteresis loop appears with the present increment $\Delta c_1 = 0.002$. We judge that a weak first-order or a second-order transition takes place there. On the other hand, for $c_2 = 0.8$, $U$ looks smooth showing no gap and hysteresis loop. Therefore we judge that no first-order transition takes place. Concerning to the possibility of a second-order transition, we check whether the peak of $C$ at $c_1 \simeq 0.58$ develops as the system size $L$ is increased [4]. Our preliminary analysis using $L = 20, 24$ shows that the size-dependence is rather weak, although the errors in $C$ are too large to draw a definitive conclusion. For a lower value $c_2 = 0.75$, $U$ and $C$ is smoother, and in particular, $C$ spreads wider than $c_2 = 0.80$. From these observation, we conclude that the line of transition should terminate at $0.75 \lesssim c_2 \lesssim 0.85$.

In Fig. 6 we show $U$ and $C$ vs. $c_2$ for $c_1 = 0.3$. $U$ has two branches that meet at $c_2 \sim 1.01$ with different slopes and a small hysteresis loop. We conclude that there is a weak first-order or a second-order transition at $c_2 \simeq 1.01$.

It is certainly true that more number of sweeps and smaller increments, $\Delta c_1$, certainly give rise to smaller errors in $U$ and $C$ and more precise determination of the location and the order of the transition points. However, the allowed size of errors in the location of the transition points drawn in Fig. 1 in the text is about $\Delta c_1 \simeq 0.02$, i.e., almost same as the size of the marks drawn there, and therefore the accuracy of the present MC study is almost sufficient for the purpose to draw Fig. 1 in the text. On the other hand, definitive determination of the order of phase transition for some points requires more detailed study by the MC simulations. We hope to report on this subject in a future publication.

[1] For more details on the present method to determine a phase structure by MC simulations, see, e.g., Refs. [25,30] cited in the text.
[2] N. Metropolis, A. W. Rosenbluth, M. N. Rosenbluth, A. Teller, E. Teller, J. Chem. Phys. 21, 1087 (1953).
[3] K. Jansen, J. Jersák, C. B. Lang, T. Neuhaus, G. Vones, Nucl. Phys. B 265, 129 (1986).
[4] According to the finite-size scaling hypothesis [See, e.g.,
L. P. Kadanoff, Physics 2, 263 (1966)], $C$ near the second-order transition point behaves for large $L$ as $C(c_1,L)/V = L^{\sigma/\nu} f(L^{1/\nu} \epsilon)$ for large $L$, where $\epsilon = (c_1 - c_{1c})/c_{1c}$ and $c_{1c}$ is the critical point for $L \to \infty$. $f$ is the scaling function, and $\sigma, \nu$ are the critical exponents.
