# Applications of Worm Algorithm for Monte Carlo Simulations of Physical Systems Described by the J-current Model

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In this document Monte Carlo simulations using worm algorithm for quantum bosonic systems mapped on classical statistical J-current model are discussed. Results of successful applications are also covered. Supplementary C++ library and examples of programs are explained.

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Materials from this document will be eventually used by the author in his Ph.D. thesis.

#### Contents

	Introduction	1
I.	J-current Model	1
	A. J-current model "derivation"	2
	1. From bosonic Hubbard model to quantum rotor model	2
	2. From quantum rotor model to classical statistical $J$ -current model	2
	B. Physical intuition	2
	C. Observables	3
II.	Worm Algorithm for $J$ -current Model	3
	A. Worm algorithm updates	3
	B. Monte Carlo procedure	3
	1. Simple isotropic model without disorder	3
	2. Exponent ratios	4
	3. Acceptance ratio	4
III.	Physical Applications	4
	A. Physical systems	4
	B. Physical phenomena	4
	1. Theory	4
	2. Simulations	5
IV.	Program Organization	5
	A. Program libraries	5
	B. Sample program	5
	C. Used data structures	5
	1. Configuration	5
Α.	Online Visualization of Worm Algorithm for	
	J-current Model	6
	1. Model	6
	a. User interface	6
	References	6

## Introduction

Full microscopic simulations of quantum systems which yield results that are in one-to-one correspondence with experimental measurements require development of first-principle simulation techniques, such as quantum Monte Carlo. However, some important information about phase transitions (e.g., critical indexes, universal jumps) can be revealed by studying model systems.

The J-current model—also called the bond-current model, or link-current model—is a classical statistical model of divergenceless currents on a lattice. It was originally developed for the study of quantum phase transitions in bosonic systems by implementing the pathintegral mapping of a d-dimensional, bosonic quantum system onto a (d+1)-dimensional classical statistical model {Wallin et~al.,~1994:~[4]} (see also § I). The J-current model describes phase transitions in a wide variety of physical systems:  ${}^4{\rm He}$  in porous media and aerogels, superfluid films on various substrates, Josephson junction arrays, granular superconductors, disordered magnets, ultracold atomic systems, etc. (see § III).

Worm algorithm {Prokof'ev and Svistunov, 2001: [3]} has proven to be an extremelly efficient for models with the configuration space of closed loops (including J-current model) by eliminating the problem of critical slowing down and providing direct Monte Carlo estimators for winding numbers and Green functions (see § II).

# I. J-CURRENT MODEL

In  $\S$  I.A I review {Wallin et al., 1994: [4]} how after set of approximations one can arrive from d-dimensional bosonic quantum Hubbard model to (d+1)-dimensional classical statistical J-current model. At large bosonic densities, when amplitude fluctuations of complex order parameter can be neglected, phase fluctuations of order parameter are only relevant at the phase transition. In this case phase transition universality class of both models is the same.

In  $\S$  I.B I relate boson-particle language with *J*-current representation. How to evaluate in *J*-current model main observables, e.g., particle density, compressibility, stiffness and Green functions, is explained in  $\S$  I.C.

{Sondhi et al., 1997: [5]} is a good complementary

introduction to the topics of this section.

## A. J-current model "derivation"

# 1. From bosonic Hubbard model to quantum rotor model

Lets consider interacting bosons on a lattice. Since one of the topics of this paper is the study of zero temperature, T=0, quantum phase transitions (QPT), it is necessary to have repulsion in order to prevent bosons from collapsing in the highly localized ground state. The simplest model will be the disordered bosonic Hubbard

$$H_{\rm bH} = H_0 - H_1,$$
 (1)

where

$$H_0 = \frac{U}{2} \sum_{\mathbf{r}} \hat{n}_{\mathbf{r}}^2 - \sum_{\mathbf{r}} (\mu + v_{\mathbf{r}} - t_0) \,\hat{n}_{\mathbf{r}},$$
 (2a)

$$H_1 = -\sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} t_{\mathbf{r}, \mathbf{r}'} \left( \hat{\Phi}_{\mathbf{r}}^{\dagger} \hat{\Phi}_{\mathbf{r}'} + \hat{\Phi}_{\mathbf{r}'} \hat{\Phi}_{\mathbf{r}}^{\dagger} \right). \tag{2b}$$

Here U is the constant soft-core on-site repulsion and  $t_0 = \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} t_{\mathbf{r}, \mathbf{r}'}$ . There is a diagonal disorder of chemical potential,  $\mu$ , varying with strength  $v_{\mathbf{r}}$  (some symmetrical distribution of  $v_{\mathbf{r}}$  centered around zero is commonly considered). There is also an off-diagonal disorder in the hopping strength  $t_{\mathbf{r}, \mathbf{r}'}$ . As usual,  $\hat{\Phi}_{\mathbf{r}}$  is the complex field,  $\hat{n}_{\mathbf{r}} = \hat{\Phi}_{\mathbf{r}}^{\dagger} \hat{\Phi}_{\mathbf{r}}$  is the number operator on the site  $\mathbf{r}$ , and  $\langle \mathbf{r}, \mathbf{r}' \rangle$  denotes summation over pairs of the nearest neighbours, each pair is counted once.

In the case of small fluctuations  $\delta n_{\mathbf{r}}$  of boson densities near large filling factor  $n_0$ , i.e.  $n_0 \gg \delta n_{\mathbf{r}}$ , approximation

$$\hat{\Phi}_{\mathbf{r}} \approx \sqrt{n_0 + \delta \hat{n}_{\mathbf{r}}} \cdot e^{i\hat{\Theta}_{\mathbf{r}}} \tag{3}$$

leads to quantum rotor model

$$H_{qr} = \frac{U}{2} \sum_{\mathbf{r}} \delta \hat{n}_{\mathbf{r}}^{2} - \sum_{\mathbf{r}} (\mu + v_{\mathbf{r}}) \, \delta \hat{n}_{\mathbf{r}}$$
$$- \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} 2n_{0} \cdot t_{\mathbf{r}, \mathbf{r}'} \cdot \cos\left(\hat{\Theta}_{\mathbf{r}} - \hat{\Theta}_{\mathbf{r}'}\right), \tag{4}$$

where  $\delta \hat{n}_{\mathbf{r}} = -\frac{1}{i} \frac{\partial}{\partial \Theta_{\mathbf{r}}}$  and phase operator  $\hat{\Theta}_{\mathbf{r}}$  are canonically conjugated operators.

Note that in original bosonic Hubbard model (1) number of particles on a site is greater or equal zero,  $n_{\bf r} \geq 0$ , while in rotor model (4) fluctuations of particles number,  $\delta n_{\bf r}$ , can take any value from  $-\infty$  to  $+\infty$ . Nevertheless, in the case  $n_0 \gg \delta n_{\bf r}$  this fact should have no effect on universality class.

# 2. From quantum rotor model to classical statistical J-current model

{Wallin et al., 1994: [4]} start with the partition function  $Z(\beta)$  of d-dimensional quantum rotor model (4) at

finite temperature,  $k_{\rm B}T = 1/\beta$ ,

$$Z(\beta) = \text{Tr}e^{-\beta H_{\text{qr}}}.$$
 (5)

Path-integral evaluation of trace leads to introduction of additional dimension of imaginary time  $\tau$  satisfying periodic boundary conditions. In discrete/lattice version, imaginary time interval  $\tau \in [0, k_{\rm B}T/\hbar]$  is sliced in M parts of size  $\Delta \tau$ .—In the case of non zero temperature,  $\Delta \tau$  corresponds to some ultraviolet cutoff. In the case of QPT, zero temperature limit  $T \to \infty$  (i.e.  $\Delta \tau \to 0$ ) and thermodynamical limit of infinite system size  $L \to \infty$  (i.e. lattice spacing  $a \to 0$ ) are related to one another. Limiting procedure must preserve dynamical-scaling  $\xi_{\tau} \sim \xi^{z}$ , where z is dynamical exponent, and  $\xi$  and  $\xi_{\tau}$  are spacial and temporal correlation lengths, respectively. This is equivalent to  $M \sim N^z$ , where N = L/a is effective linear spacial lattice size.—Finally, using Villian approximation one arrives to classical statistical (d+1)-dimensional Jcurrent model of integer bond currents

$$Z_J(\beta) = \sum_{\{\mathbf{J}\}}^{\nabla \cdot \mathbf{J} = 0} e^{-\beta H_J}, \tag{6}$$

where classical J-current Hamiltonian is

$$\beta H_J = \sum_{\mathbf{n},\alpha} \left[ \frac{K_{\mathbf{n},\alpha}}{2} J_{\mathbf{n},\alpha}^2 - \Delta \tau (\mu + v_{\mathbf{r}}) J_{\mathbf{n},\tau} \right]. \tag{7}$$

Summation in (6) is taken over divergenceless J-current configurations. Anisotropic along  $\tau$ -direction strengths of interactions are given by

$$\exp\left(-\frac{K_{\mathbf{n},\langle\mathbf{r},\mathbf{r}'\rangle}}{2}\right) = \frac{t_{\langle\mathbf{r},\mathbf{r}'\rangle} \cdot \Delta\tau}{2}, \tag{8a}$$

$$K_{\mathbf{n},\tau} \equiv K_{\tau} = U \cdot \Delta \tau.$$
 (8b)

Integer  $J_{\mathbf{n},\alpha}$  is a current component from site  $\mathbf{n}=(\mathbf{r},\tau)$  in direction  $\alpha$  on the corresponding bond of (d+1)-dimensional lattice. In the case of general topology of underlying lattice  $\alpha=\{\langle\mathbf{r},\mathbf{r}'\rangle,\tau\}$ . From now on I will work only with hypercubic spacial lattices because in all transitions considered in this paper changes in the symmetry of spacial lattice are not expected to modify critical behaviour. This fact allows me to adopt simplified notation, see Table I.

Zero-divergence constrain, i.e. (d+1)-dimensional continuity equation, is

$$\sum_{\alpha} (J_{\mathbf{n},\alpha} + J_{\mathbf{n},-\alpha}) = 0. \tag{9}$$

# B. Physical intuition

to be typed

# C. Observables

I will not repeat here scaling arguments of {Wallin et al., 1994: [4]}. I will only state final formulas for representation of physical observables in J-current model. (Microscopic details are unimportant for universal scaling. Thus, it is convenient to set lattice spacing, a and  $\hbar \Delta \tau$ , to unity.)

Winding number  $m_{\alpha}$  in  $\alpha$ -direction, or number of twists, is defined as

$$m_{\alpha} = \frac{1}{L_{\alpha}} \sum_{\mathbf{n}} J_{\mathbf{n},\alpha}.$$
 (10)

Physical meaning of  $m_{\tau} > 0$  and  $m_{\tau} < 0$  is total number of particles and holes in the system, respectively.

Superfluid stiffness  $\rho$  is given by

$$\rho = \frac{1}{L^{d-2}L_{\tau}} \cdot \frac{1}{d} \sum_{\alpha=1,\dots,d} \langle m_{\alpha}^2 \rangle. \tag{11}$$

Compressibility  $\kappa$  is given by

$$\kappa = \frac{1}{L^{d-2}L_{\tau}} \cdot \left[ \langle m_{\tau}^2 \rangle - \langle m_{\tau} \rangle^2 \right]. \tag{12}$$

#### II. WORM ALGORITHM FOR J-CURRENT MODEL

## A. Worm algorithm updates

There are two possible types of updates

**jump:** Starting with a zero-divergent configuration select a site in (d+1)-dimensional lattice to hatch the smallest possible zero size worm by placing its head and tail simultaneously into this site.

**move:** Grow worm head from a site  $\mathbf{n}$  to its neighbour on (d+1)-dimensional coordinate-time lattice. Current on the corresponding bond will be "increased" by 1 according to the rules below:

$$\odot \leftarrow \circledast \cdots \odot \equiv J_{\mathbf{n} - \hat{\alpha} \alpha} - 1 = -(J_{\mathbf{n} - \alpha} + 1) . (14)$$

direction: 
$$\alpha = \{1, \dots, d, d+1\} \equiv \{x, y, z, \tau\} \equiv \{r, \tau\}$$
  
unit vector:  $\hat{\alpha} = \{\hat{x}_1, \dots, \hat{x}_d, \hat{x}_{d+1}\} \equiv \{\hat{x}, \hat{y}, \hat{z}, \hat{\tau}\} \equiv \{\hat{\mathbf{r}}, \hat{\tau}\}$   
lattice site:  $\mathbf{n} = \{x_1, \dots, x_d, x_{d+1}\} \equiv \{x, y, z, \tau\} \equiv \{\mathbf{r}, \tau\}$   
lattice size:  $L_{\alpha} = \{L_1, \dots, L_d, L_{d+1}\} \equiv \{L, L, L, L_{\tau}\}$ 

TABLE I Notation for (3+1)-dimensional hypercubic lattice. From the context it will be obvious to distinguish between usage of the same characters in definition of  $\alpha$  and  $\mathbf{n}$ . Moreover, if, for example, there is no need to specify spacial coordinate of a site, I will use  $\mathbf{r}$  instead of (x,y,z). By definition,  $-\alpha$  direction is understood as opposite to  $\alpha$ .

Such updating procedures are enough to fulfil ergodicity of the algorithm, i.e. it is possible to create any "worm" current configuration—just one need to "disconnect" head of worm from its tail at a right site and to move head in a right direction, see Fig. 2.

# B. Monte Carlo procedure

# 1. Simple isotropic model without disorder

In order to illustrate algorithm, lets consider simple (d+1)-dimensional isotropic case of J-current model without disorder

$$\beta H = \frac{1}{K} \sum_{\mathbf{n},\alpha} \left( \frac{1}{2} J_{\mathbf{n},\alpha}^2 - \delta_{\alpha,\tau} \cdot \mu_{\mathbf{x}} J_{\mathbf{n},\alpha} \right). \tag{15}$$

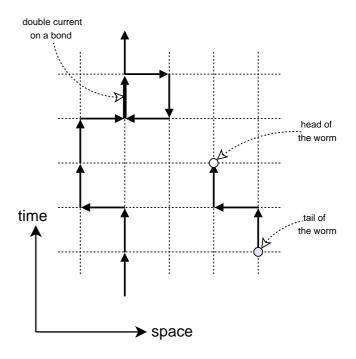


FIG. 1 Example of an extended/worm-type J-current configuration.

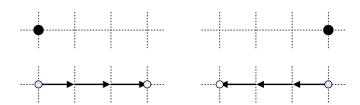


FIG. 2 Left and right set of diagrams represents how by hatching worm (filled circle) at different sites one can acquire worm digging in different directions and at a same time spanning same sites.

## 2. Exponent ratios

For the space direction move update (13) and (14) one has corresponding ratios:

$$\frac{e^{-\beta H^{new}}}{e^{-\beta H^{new}}} = \exp\left[-\frac{1}{2K}\left(\left(J_{\mathbf{n},\alpha} + 1\right)^2 - J_{\mathbf{n},\alpha}^2\right)\right] = \exp\left[-\frac{1}{K}\left(J_{\mathbf{n},\alpha} + \frac{1}{2}\right)\right], \tag{16}$$

$$\frac{e^{-\beta H^{new}}}{e^{-\beta H^{new}}} = \exp\left[-\frac{1}{2K}\left(\left(J_{\mathbf{n}-\alpha,\alpha} - 1\right)^2 - J_{\mathbf{n}-\hat{\alpha},\alpha}^2\right)\right] = \exp\left[-\frac{1}{2K}\left(\left(J_{\mathbf{n},\alpha} + 1\right)^2 - J_{\mathbf{n},-\alpha}^2\right)\right] = \exp\left[-\frac{1}{K}\left(J_{\mathbf{n},\alpha} + \frac{1}{2}\right)\right]. \tag{17}$$

This shows that one can carry out in a uniform fashion space move update, and this fact has inspired the particular choice of configuration data structure for a program—namely, for each site  $\mathbf{n}$  to store in array both  $J_{\mathbf{n},\alpha}$  and  $J_{\mathbf{n},-\alpha}$ , see § IV.C.1 and Eq. (23).

For the time direction move update (13) and (14) one has corresponding ratios:

$$\frac{e^{-\beta H^{new}}}{e^{-\beta H^{new}}} = \exp\left[-\frac{1}{K}\left(J_{\mathbf{n},\alpha} + \frac{1}{2}\right) + \frac{+\mu_{\mathbf{x}}}{K}\right], \quad (18)$$

$$\frac{e^{-\beta H^{new}}}{e^{-\beta H^{new}}} = \exp\left[-\frac{1}{K}\left(J_{\mathbf{n},-\alpha} + \frac{1}{2}\right) + \frac{-\mu_{\mathbf{x}}}{K}\right]. \quad (19)$$

For shortening of notation introduce

$$\mu_{\mathbf{x},+\tau} = -\mu_{\mathbf{x},-\tau} \equiv \mu_{\mathbf{x}},\tag{20}$$

then ratios for a move in arbitrary direction  $\alpha$  or  $-\alpha$  in Eqs. (16,17,18,19) will be represented by a single formula

$$\frac{e^{-\beta H^{new}}}{e^{-\beta H^{old}}} = \exp\left[-\frac{1}{K}\left(J_{\mathbf{n},\alpha} + \frac{1}{2}\right) + \delta_{\alpha,\pm\tau} \cdot \frac{\mu_{\mathbf{x},\tau}}{K}\right]. \tag{21}$$

# 3. Acceptance ratio

to be written

# **III. PHYSICAL APPLICATIONS**

WA for the J-current model bridged the gap between analytical methods and simulations of phase transitions in systems of interacting bosons with or without disorder (see  $\S$  III.A). WA has proven to be a useful numerical

tool in confirming the validity of analytical methods and hypothesis for describing and predicting the underlying, non-trivial physics of phase transitions in bosonic systems (see § III.B).<sup>2</sup>

# A. Physical systems

Bosonic Hubbard model and quantum rotor model cover wide range of interacting bosonic-type systems. For many of them conditions of validity of the J-current model "approximation" are satisfied. As a result, this allows one to correlate WA simulations of the J-current model with physical phenomena in such systems as  $^4{\rm He}$  in porous media and aerogels, superfluid films on various substrates, Josephson junction arrays, granular superconductors, disordered magnets, ultracold atomic systems, etc.

# B. Physical phenomena

Also see list of related publications at http://montecarlo.csi.cuny.edu/umass/publications.html.

# 1. Theory

1. {Fisher et al., 1989: [6]} – "Boson Localization and the Superfluid–Insulator Transition"

<sup>&</sup>lt;sup>1</sup> In a same fashion cluster algorithm for the Potts/Ising model {Swendsen and Wang, 1987: [2]} has successfully complemented research in the field of spin systems.

One need to keep in mind that in this paper only universal properties of phase transitions are discussed. For these purposes it is sufficient to consider approximate classical statistical J-current model that preserves universality class of original quantum mechanical bosonic model. It would be unjustified to implement for these purposes such exact techniques as quantum Monte Carlo method, for example, see {Ceperley, 1999: [1]} and references therein.

2. {Prokof'ev and Svistunov, 2005: [7]} – "Supersolid State of Matter"

# 2. Simulations

- {Alet and Sørensen, 2004: [8]} "Generic incommensurate transition in the two-dimensional boson Hubbard model"
- {Prokof'ev and Svistunov, 2004: [9]} "Superfluid— Insulator Transition in Commensurate Disordered Bosonic Systems: Large-Scale Worm Algorithm Simulations"
- 3. {Burovski et~al., 2005: [10]} "Superfluid Interfaces in Quantum Solids"
- 4. {Kuklov et al., 2004: [11]} "Superfluid–Superfluid Phase Transitions in a Two-Component Bose-Einstein Condensate"
- 5. {Kuklov et al., 2004: [12]} "Commensurate Two-Component Bosons in an Optical Lattice: Ground State Phase Diagram"
- 6. {Kuklov et al., 2004: [13]} "Weak First-Order Superfluid–Solid Quantum Phase Transitions"
- {Balabanyan et al., 2005: [14]} "Superfluid-Insulator Transition in Commensurate One-Dimensional Bosonic System with Off-Diagonal Disorder"

Note that simulation 1 from this list were carried with recently proposed geometrical WA {Alet and Sørensen , 2003: [15]}.

# IV. PROGRAM ORGANIZATION

Program archive at http://montecarlo.csi.cuny.edu/umass/WAJCM.zip contains repository of libraries (see  $\S$  IV.B) and program example with instructions for its compilation.

In § IV.C.1 explicitly configurational data-array representation is related with pictorial one.

# A. Program libraries

Self explanatory inline commented libraries structured in two folders: BIBLIO/ PROGRAMS/worm-main/. The first folder holds supplementary functions, e.g., safe array initializations, exception handling, etc. In the second folder main classes are placed.—structures.h deals with parameters, configurations and statistics, sysworm.h describes wrapping simulation class and modifying allh.h one sets different compilation options.

It is important to note that lattice topology, e.g., dimensionality, maximum value of current on a bond, etc., is set through BIBLIO/wnamespace.h.

## B. Sample program

Follow skeleton of the sample program from archive starting to build your own application.

# C. Used data structures

# 1. Configuration

One deals with a square  $D \equiv (d+1)$ -dimensional lattice of size  $L_1 \cdots L_d \cdot L_\tau \equiv L^d \cdot L_\tau$ . An integer vector  $\mathbf{n} = (\mathbf{r}, \tau)$  labeling some site is encoded in a single number<sup>3</sup>

$$\mathbf{n} \cong x_1 + L_1 \cdot x_2 + L_1 \cdot L_2 \cdot x_3 + L_1 \cdots L_d \cdot \tau. \tag{22}$$

[C++ indexing is adopted, e.g.  $0 \le x_1 < L_1$ .] There is an integer current  $J_{\mathbf{n},\alpha}$  on a bond adjacent to the site  $\mathbf{n}$  along  $\alpha$  direction (see also Table I).

**Note:** for the broken bond I attribute current in the corresponding direction to be equal to the "special" number 127. Occasionally, this limits simulation to have values of currents to be in range  $-127 \le J \le 127$ .

Minimal size of array to hold current configuration is  $D \cdot L^d T$ . Current in  $-\alpha$  direction at a given site can be calculated from its neighbours' current in  $\alpha$  direction  $J_{\mathbf{n}-\hat{\alpha},\alpha} = -J_{\mathbf{n},-\alpha}$ . But, I sacrifice memory in favor of decreasing amount of repetitive/unnecessary calculations in Monte Carlo procedure. Thus, I have array of  $2D \cdot L^d T$  size, where for a given site  $\mathbf{n}$  starting at position  $2D \cdot \mathbf{n}$  full information for the values of current in 2D directions is located. Following order of currents in 2D directions  $\{0,1,\ldots,2D-1\}$  from a given site  $\mathbf{n}$  is adopted

$$\{J_{\mathbf{n},-x} \mid J_{\mathbf{n},x} \mid \dots \mid J_{\mathbf{n},-\tau} \mid J_{\mathbf{n},\tau}\}. \tag{23}$$

In other words, for a given site **n** value of current in negative direction precedes value of current in corresponding positive direction, see Fig. 3.

According to WA theory of § II, closed loop configurations are the one that correspond to real physical state

$$\tau = \mathbf{n}/L^d \quad and \quad \mathbf{n} - = L^d \cdot \tau,$$
 
$$x_d = \mathbf{n}/L^{d-1} \quad and \quad \mathbf{n} - = L^{d-1} \cdot x_d,$$
 
$$\dots$$
 
$$x_2 = \mathbf{n}/L \quad and \quad \mathbf{n} - = L \cdot x_2,$$
 
$$x_1 = \mathbf{n}.$$

DIR = PosDIR/2 — real move D-direction,

 $\begin{array}{ll} \texttt{MOVE= PosDIR\%2} \longrightarrow \text{on which side to move } 0: [\leftarrow] \text{ and } +1: [\rightarrow], \\ \texttt{SIGN= 2*MOVE-1} \longrightarrow \text{sign of move } -1: [\leftarrow] \text{ and } +1: [\rightarrow], \end{array}$ 

(PosDIR - SIGN) — opposite 2D-direction to PosDIR.

 $<sup>^3</sup>$  back transformation from a single number  ${\bf n}$  to a set of D coordinates is straightforward

<sup>&</sup>lt;sup>4</sup> In order to save time in generating a direction of the next move in Monte Carlo procedure, generate only one random integer PosDIR=rndm(2D) and then convert it into

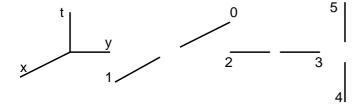


FIG. 3 Example of indexing of directions in (2+1)D case.

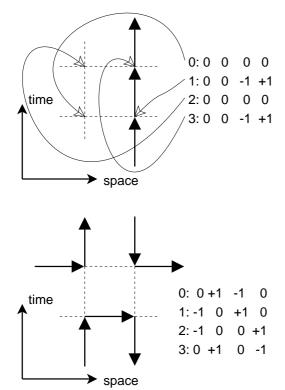


FIG. 4 Examples of configurations for  $2\times 2$  system. Lines represent sites numbered/ordered according to (22) and each line holds information about outgoing currents from the site according to (23) indexing.

of the system. Thus, my Monte Carlo procedure iterates from one of closed loop configurations to another. (Of course, some statistics, e.g., Green functions, are collected from the states of the system in extended configurations, but only closed loop configurations are save, check, etc.) See Fig. 4 for examples.

# APPENDIX A: Online Visualization of Worm Algorithm for J-current Model

P. Ivanushkin provided online cartoon like visualization of WA updating extended configurational space of J-current model, see http://montecarlo.csi.cuny.edu/umass/.

# 1. Model

For an illustrationary purposes, isotropic (1+1)-dimensional case of J-current model for the system of size  $10 \times 10$  without disorder is considered. Explicit form of hamiltonian (15) is

$$\beta H = \frac{1}{K} \sum_{\mathbf{n} = (x,\tau)} \left[ \frac{1}{2} \left( J_{\mathbf{n},\hat{x}}^2 + J_{\mathbf{n},\hat{\tau}}^2 \right) - \mu J_{\mathbf{n},\hat{\tau}} \right].$$
 (A1)

# a. User interface

User is given an option to choose K and  $\mu$  or select preset values (phase diagram for model (A1) is provided). Also, in addition to blank J-current configuration, several other configurations are provided for a choice of initial configuration for WA simulation.

Finally, user can view/save snapshots of extended *J*-current configurations after each update of WA in interactive regime or can view/save continuous movie.

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