Conformal invariance and a quantum Monte Carlo method

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• Introduction

- Conformal mappings
- Critical phenomena
- Conformal invariance
- Monte Carlo simulations
- A quantum Monte Carlo method
- Numerical results
- Conclusions

Conformal mappings

• Definition: A conformal mapping $\vec{r} \rightarrow \vec{r}' = \vec{r}'(\vec{r})$

 \iff infinitesimal objects keep their shape.

• Examples:



 $z' = \ln z = \ln(x + iy)$



(1) Cardy's mapping (2) Inversion transformation

$$z' = 1/z$$



‡ For d = 2, any <u>analytical</u> complex function is conformal

‡ Mapping (4) can be generalized to the surface of a spheroid (Y.J. Deng and H.W.J. Böte, Phys. Rev. E 036107, 2003).

Mappings (1) and (2) \Rightarrow *flat* geometries; mappings (4) and (3) \Rightarrow *curved* geometries or curved boundaries



Cardy's mapping for d = 3

‡ Surface of the 4D cylinder is named a <u>spherocylinder</u> (Y.J. Deng and H.W.J. Böte, Phys. Rev. Lett. 190602, 2002).



By M.E. Escher (1898-1972, Holland)







(3)

By H. Lenstra, B. de Smit *et. al* (Leiden University) (See. *e.g., New York Times* July 30, 2002)

Critical phenomena

• Examples:



Liquid-gas transition Ferro-paramagnet transition

Near T_c : Specific-heat $C \propto |T - T_c|^{-\alpha}$

Susceptibility $\chi \propto |T-T_c|^{-\gamma}$

 $\ddagger \alpha, \gamma$ take same values: same universality class

• Theoretical descriptions

Ising model

 $\mathcal{H}/k_{\mathsf{B}}T = -K\sum_{\langle i,j \rangle} s_i s_j$, $(s_i = \pm 1, K : interactions)$

q-state Potts model

$$\mathcal{H}/k_{\mathsf{B}}T = -K\sum_{\langle i,j
angle} \delta_{\sigma_i\sigma_j} , \qquad (\sigma_i = 1, 2, \cdots, q)$$

Conformal invariance

- For d = 2, conformal field theory has <u>predicted</u> a series of critical exponents for Potts models.
- At criticality, under a conformal mapping,

 $\langle \varphi_1(\vec{r}_1)\varphi_2(\vec{r}_2)\cdots\rangle_{\vec{r}} = \\ b(\vec{r}_1)^{-X_1}b(\vec{r}_2)^{-X_2}\cdots\langle \varphi_1(\vec{r}_1')\varphi_2(\vec{r}_2')\cdots\rangle_{\vec{r}'}$

- φ_i : scaling operators (*m*, *e* etc),
- X_i : scaling dimensions (related to $lpha,\gamma,\cdots$),
- $b(\vec{r})$: scaling factor $(b(\vec{r})^d = \det(\partial \vec{r} / \partial \vec{r'}))$

‡ Examples:

- (1) Along (sphero)cylinder ($|u| \gg 1$)
 - $\langle \varphi(0)\varphi(u)
 angle \propto \exp\left(-|u|/\xi_R
 ight), \quad \xi_R=R/X$

(2) On surface of a sphere

 $\langle \varphi(0,0) \varphi(heta,\psi)
angle \propto \sin^{-2X}(heta/2)$

(3) On interior of a circle

 $\langle arphi(r)
angle \propto [1-(r/R)^2]^{-X}$

‡ <u>Difficulties</u>:

(1) Can one numerically verify these assumptions?

(2) How can one simulate such curved geometries?

 Δ <u>Solution</u>: Make use of a quantum Hamiltonian and develop a quantum Monte Carlo method.

Monte Carlo simulations

Boltzmann distribution: $w \propto \exp(-E/k_{\rm B}T)$

• Metropolis algorithm



1, choose a spin s_i , and 2, calculate ΔE as $s_i \rightarrow -s_i$ 3, draw random number $0 \le r < 1$, if $r < e^{-\Delta E/k_b T}$, then $s_i \rightarrow -s_i$; else, do nothing

suffer from critical slowing down

Swendsen-Wang and Wolff cluster algorithm

spin up-down ($\uparrow\downarrow$) symmetry

Geometric cluster algorithm

spatial geometry (inversion invariance) (H.W.J. Böte and J.R. Heringa, Phys. Rev. E **57** 4976, 1997)

A quantum Monte Carlo method

• Classical Ising model on $N \times M$ square lattice:

$$\mathcal{H}/k_{\mathsf{B}}T = -\sum_{i}^{N}\sum_{j}^{M} [K_{x}s_{i,j}s_{i+1,j} + K_{y}s_{i,j}s_{i,j+1}],$$

Take *anisotropic* limit $\epsilon \rightarrow 0$:

$$K_y = \epsilon/t$$
, $\exp[-2K_x] = \epsilon$, (t:temperature-like)

• Quantum transverse Ising chain

$$\mathcal{H}_Q = -\sum_{i}^{N} (s_i^z \sigma_{i+1}^z + t \sigma_i^x), \ (\sigma^z, \sigma^x : \text{Pauli matrices}).$$

t: transverse field, criticality at: $t_c = 1$.

• A continuous Wolff algorithm (H.W.J. Böte and Y.J. Deng, Phys. Rev. E 066110, 2002)

[Difficulty] For $\epsilon \to 0$, $M \sim 1/\epsilon$, since $\xi_x \sim 1/\epsilon$

[Solution] Rescale *x*-coordinate

 $\downarrow \quad x' = x/\epsilon$

x-dimension continuous

Dynamical variables: \pm interfaces



Procedures of rescaling



A Wolff cluster





Quantum criticality

Simulations of a d = 2 quantum spin model as viewed from the so-called imaginary time direction. The critical clusters are essentially fractal in nature.

By Y.J. Deng, J.R. Heringa, and H.W.J. Böte

(see e.g. http://www.fom.nl)

• simulations on a sphere



Numerical results

• Critical points
$$(d = 2)$$
:
 $t_c = 3.04438(2)$: quantum transverse Ising model
 $t_c = 4.3233(1)$: quantum transverse percolation model

• Simulations on sphere and disc geometries (d = 1): Ising: $X_h = 0.12496(9)$ (conformal invariance)

 $X_t = 0.996(6)$

 $X_h = 1/8$, $X_t = 1$ (exact solutions)

Percolation: $X_h = 0.10420(5)$ (conformal invariance)

 $X_h = 5/48 \approx 0.10416 \cdots$ (exact solutions)

• Simulations on spherocylinder (d = 2)

Ising: $X_h = 0.5178(6)$ (conformal invariance)

 $X_t = 1.419(7)$

 $X_h = 0.5184(1), X_t = 1.4132(3)$ (other sources)

Percolation: $X_h = 0.479(1)$ (conformal invariance)

 $X_h = 0.476(4)$ (other sources)



- We have verified assumptions of conformal invariance in curved geometries.
- We show that conformal invariance is also a powerful tool to study critical phenomena for d = 3.
- We have developed an efficient Monte Carlo algorithm for descrete quantum spin models.