Application of the Coherent Anomaly Method to 1/d Expansions for a Self-Interacting Self-Avoiding Lattice Walk

Takao Ishinabe
Faculty of Engineering, Yamagata University
Yonezawa 992, Japan

1. Introduction

Fisher and Gaunt[1] first established the 1/d expansion method for a self-avoiding walk (SAW) on a d-dimensional lattice. The 1/d expansion for the free energy amolitude of SAW has been given by Gaunt[2] through $O(d^{-5})$. Recentry, Nemirovsky et al[3,4] have developed more general 1/d expansions for SAW with the aid of the lattice cluster theory using the exact enumeration data of $C_{n,m}$ and $R_{n,m}$ in d = 2 - 6, where $C_{n,m}$ and $R_{n,m}$ are the number of n-step walks and the mean square end-to-end distance with m internal contacts, respectively. Here we estimate the exponents γ and ν for SAW and θ' chain (the definition of θ' will be given later) by combining the 1/d expansions with the coherent anomaly method (CAM)[5].

2. 1/d expansions

The partition function of the chain with nearest-neighbor interaction ε is written as

$$C_n(\omega) = \sum_{m=0} C_{n,m} e^{m\omega} \tag{1}$$

where $\omega = -\varepsilon/kT$. We assume

$$C_n(\omega) \cong A_C(\omega) \; n^{\gamma(\omega)-1} \mu(\omega)^n \tag{2}$$

and define the reduced free energy by

$$F^*(\omega) \equiv \log \mu(\omega) = \lim_{n\to\infty} n^{-1} \log C_n(\omega) \tag{3}$$

Putting $\gamma = 1$ in (2) and $f = e^{\omega} - 1$, we have[3]

$$F^*(f) = \log\sigma + f\sigma^{-1} - (1 - f - 3/2\, f^2)\sigma^{-2} - (2 - 7f - 11f^2 - 16/3\, f^3)\sigma^{-3} - (23/2 - 35f - 117/2\, f^2 - 56f^3 - 103/4\, f^4 - 3f^5)\sigma^{-4} - (64 - 250f - 251f^2 - 532f^3 - 379f^4 - 626/5\, f^5 - 14f^6)\sigma^{-5} - \dots \quad (4)$$

and the free energy amplitude

$$A_C(f) = (1 + \sigma^{-1})\{1 - 2f\sigma^{-1} + (3 - 8f - 6f^2)\sigma^{-2} + (13 - 70f - 75f^2 - 28f^3)\sigma^{-3} + (107 - 588f - 685f^2 - 456f^3 - 161f^4 - 18f^5)\sigma^{-4} + (895 - 5818f - 5192f^2 - 6018f^3 - 3417f^4 - 988f^5 - 112f^6)\sigma^{-5} + \dots\} \quad (5)$$

where $\sigma = 2d - 1$. Similarly, we obtain[4]

$$A_R(f) = 1 + (2 - 2f)\sigma^{-1} + (6 - 14f - 4f^2)\sigma^{-2} + (28 - 102f - 68f^2 - 22f^3)\sigma^{-3} + (180 - 832f - 712f^2 - 412f^3 - 134f^4 + 23f^5)\sigma^{-4} + (1382 - 6700f - 10142f^2 - 12312f^3 - 16658f^4 - 11654f^5 - 1441f^6)\sigma^{-5} + \dots \quad (6)$$

on the basis of the assumption

$$R_n^2(f) \cong A_R(f)\, n^{2\nu(f)} \quad (7)$$

with $\nu = 1/2$.

The 1/d expansions (5) and (6) seem[3,4] to diverge with increasing in the order of expansions for small d. This suggests[6] we can estimate γ and ν by applying the CAM theory[5] to these equations since they are based on the mean-field approximation.

3. Estimation of γ and ν from CAM

The susceptibility χ of the Ising model near the critical point T_c can be written as

$$\chi \sim \varepsilon^{-\gamma} \tag{8}$$

with $\varepsilon = (T - T_c)/T_c$. The CAM theory states

$$\chi \cong \overline{\chi}(\overline{T}_c)\overline{\varepsilon}^{\ -1} \tag{9}$$

where $\overline{\varepsilon} = (T - \overline{T}_c)/\overline{T}_c$ ($\overline{T}_c$: the mean-field value of T_c), and $\overline{\chi}(\overline{T}_c)$ represents the mean-field approximation of χ given by

$$\overline{\chi}(\overline{T}_c) \sim 1/(\overline{T}_c - T_c)^{\gamma-1} \tag{10}$$

Taking the mean-field value $\gamma = 1$ in (2), we have the generating function of C_n for SAW (f = 0):

$$\chi_0 = 1 + \sum_{n=1}^{\infty} C_n x^n \cong A_C(\sigma)(1 - \mu x)^{-1} \tag{11}$$

μ being the connective constant of SAW. Since μ corresponds[1] to T_c, the comparison of (11) with (9) yields

$$A_C(\overline{\mu}) \sim (\overline{\mu} - \mu)^{-\psi} \tag{12}$$

where $\psi = \gamma - 1$ and $\overline{\mu}$ is the mean-field value of μ. Similarly, the correlation length ξ scales near T_c as

$$\xi \sim \varepsilon^{-\nu} \tag{13}$$

Since ξ and ε correspond[7] to R_n and n^{-1} for SAW, respectively, we have by comparing (13) with (7):

$$A_R(\overline{\mu}) \sim (\overline{\mu} - \mu)^{-\lambda} \tag{14}$$

where $\lambda = 2\nu - 1$.

We can estimate ψ and λ for any f using (5) and (6) provided the exact μ and some systematic mean-field values μ_n (n = 0, 1, ...) are available. If we define μ_n by

$$\mu_n(f) = \sigma \sum_{i=0}^{n-1} a_{i+1}(f)\sigma^{-i} \tag{15}$$

with $\mu_1 = \sigma$, the coefficient a_i can be determined from (4) since $F^*(f) = \log \mu(f)$. We define θ' chain by $f = \sigma^{-1}$; the θ' state is near to the theta point $\omega_\theta = 1/(\sigma - 1)$ given by the lattice model[8] in larger d. We have the systematic μ_n $(n \leqq 6)$ for SAW and θ' chain from

$$\mu_6(0) = \sigma(1 - \sigma^{-2} - 2\sigma^{-3} - 11\sigma^{-4} - 62\sigma^{-5}) \tag{16a}$$

and

$$\mu_6(\sigma^{-1}) = \sigma(1 - \sigma^{-3} - 3\sigma^{-4} - 18\sigma^{-5}) \tag{16b}$$

respectively. We plot $\log \mu_n$ against n^{-1} and extrapolate to $n \to \infty$ to determine μ_∞; the example for SAW in d = 3 is given in Fig. 1. This μ_∞ is regarded as μ in this case. We can estimate ψ and λ, i.e. γ and ν from the plots of $\log A_R(\mu_n)$ and $\log A_R(\mu_n)$ vs. $\log \Delta\mu_n$, where $\Delta\mu_n = \mu_n - \mu$, as shown in Figs. 2 and 3, respectively. The result thus obtained for SAW and θ' chain are: $\gamma_{SAW} = 1.22$ (3d), 1.06 (3.5d), 1.018 (4d) and $2\nu_{SAW} = 1.23$ (3d), 1.07 (3.5d), 1.023 (4d); $\gamma_{\theta'} = 1.026$ (3d), 1.007 (3.5d) 1.0017 (4d) and $2\nu_{\theta'} = 1.037$ (3d), 1.011 (3.5d) and 1.0031 (4d).

This estimation is ineffective for d = 2 since the determination of μ_∞ is difficult. The values of γ and 2ν for d = 3.5 are in accord with those from the exact enumeration[9]: $\gamma = 1.07 \pm 0.015$ and $2\nu = 1.07 \pm 0.01$ while those for d = 3 are somewhat larger than the expected ones. These estimates for θ' chain are almost consistent with $\gamma = 2\nu = 1$ at $d = d_c$; the marginal critical dimension d_c is three for θ chain[10].

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References

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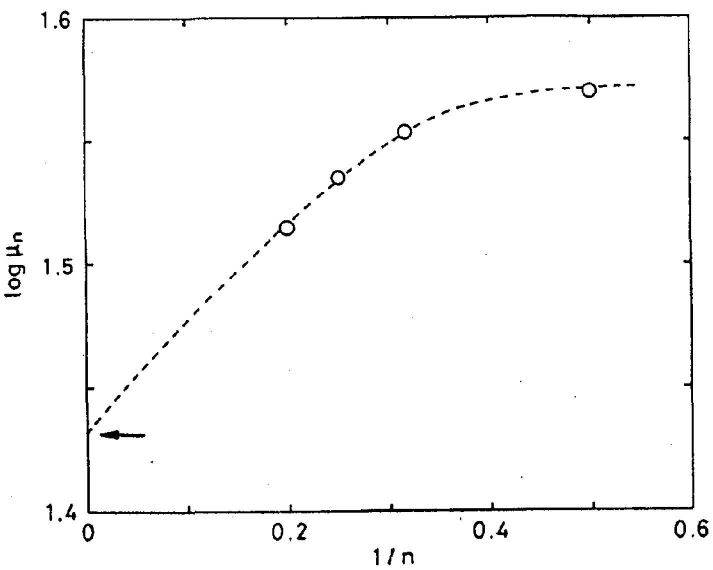

Fig.1. Estimation of μ_∞ for SAW in d = 3; the arrow indicates log μ_∞ = 1.43.

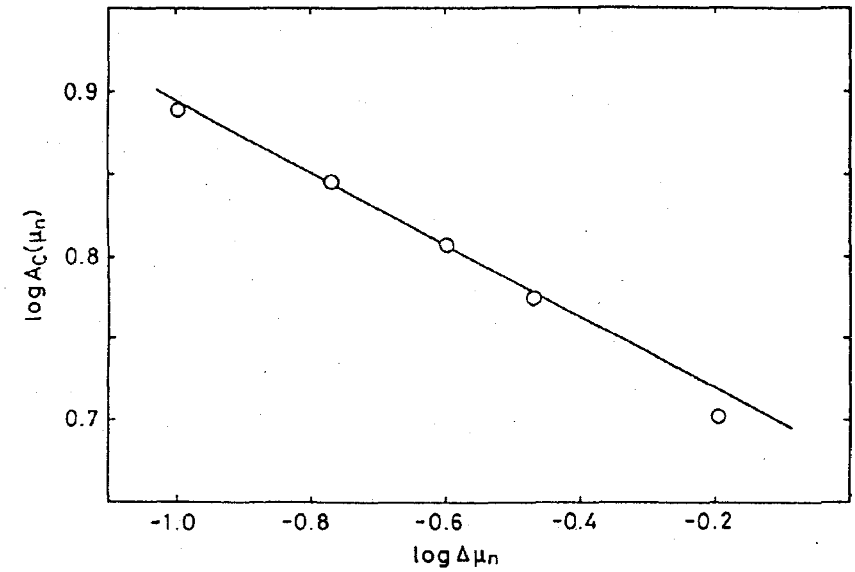

Fig.2. The plot of log $A_C(\mu_n)$ vs log $\Delta\mu_n$ for SAW in d = 3; the slope gives ψ = 0.222.

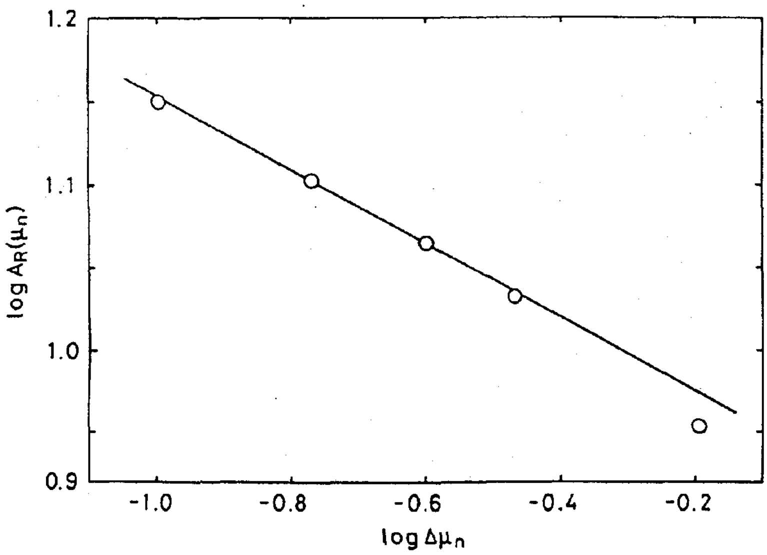

Fig.3. The same as Fig.2 but for A_R; the slope gives λ = 0.234.