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HOW GOOD IS THE VILLAIN APPROXIMATION?*

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Motivated by recent Monte Carlo confirmation that the phase transition in the U(1) lattice gauge model in $D = 4$ dimensions and its Villain approximation are of different order, we perform a quantitative analysis of this approximation. For completeness we also treat the case of the classical planar spin model (XY model) in $D = 2$ and 3 dimensions. We show the approximation is good only for *low* β and fails badly for larger β, for which it is often derived. We point out that it is an extremely accurate approximation for *all* β for a model with mixed action $\beta \cos\theta + \gamma \cos 2\theta$ and β, γ related to Villain's β_V by $\beta_V = -[2 \log I_1^\gamma(\beta)/I_0^\gamma(\beta)]^{-1}$, $I_2^\gamma(\beta)/I_0^\gamma(\beta) = (I_1^\gamma(\beta)/I_0^\gamma(\beta))^4$ where $I_b^\gamma(\beta) = \int_{-\pi}^{\pi}(\mathrm{d}\theta/2\pi)\cos b\theta\, \mathrm{e}^{\beta\cos\theta + \gamma\cos 2\theta}$ are extensions of the modified Bessel functions.

In planar spin and U(1) lattice gauge models, the Villain approximation [1] has become a favorite tool for analyzing defect structures and phase transitions. The approximation is usually inferred [2] from the obvious fact that for large β, $\exp(\beta\cos\theta)$ should be indistinguishable from the periodic gaussian which has the minima at the same places $\theta = 2\pi n$ with the same curvatures

$$\mathrm{e}^{\beta\cos\theta} \underset{\beta\to\infty}{\longrightarrow} \mathrm{e}^{\beta} \sum_{n=-\infty}^{\infty} \mathrm{e}^{-\frac{1}{2}\beta(\theta-2\pi n)^2}. \tag{1}$$

Alternatively, one finds the statement [3] that, in the Fourier expansion

$$\mathrm{e}^{\beta\cos\theta} = \sum_{b=-\infty}^{\infty} I_b(\beta)\mathrm{e}^{ib\theta},$$

one can replace the modified Bessel function by its asymptotic behavior

$$\frac{I_b(\beta)}{I_0(\beta)} \underset{\beta\to\infty}{\longrightarrow} \mathrm{e}^{-b^2/2\beta}. \tag{2}$$

While this limit is certainly true, it will be seen to be irrelevant as far as the

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application of the approximation to phase transitions is concerned. These always take place for small $\beta \lesssim 1$. This lies more in the threshold regime of the Bessel function, where

$$\frac{I_b(\beta)}{I_0(\beta)} \underset{\beta\to 0}{} \frac{1}{|b|!} \mathrm{e}^{\log(\beta/2)|b|}.$$

For small enough β, this can be replaced by

$$\frac{I_b(\beta)}{I_0(\beta)} \xrightarrow[\beta\to 0]{} \mathrm{e}^{-(1/2[-2\log(\beta/2)]^{-1})b^2} \equiv \mathrm{e}^{-b^2/2\beta_V}, \tag{3}$$

i.e. we find again a gaussian necessary for a Villain approximation, but with a redefinition of the temperature $\beta \to \beta_V = [-2\log(\beta/2)]^{-1}$. The limit (3) is making a mistake only for $|b| \geqslant 2$ where the expression is anyhow extremely small. We shall see immediately that it is this limit of the Bessel functions which is exploited by the Villain approximation, rather than (2).

It is worth recalling that Villain himself gave a prescription for his approximation which is valid in the limit of *large*, *as well as small*, β. He approximated $\mathrm{e}^{\beta\cos\theta}$ by a periodic gaussian with an unknown normalization $R_V(\beta)$ and a rescaled inverse temperature $\beta_V(\beta)$ as follows

$$\mathrm{e}^{\beta\cos\theta} \approx R_V(\beta) \sum_n \mathrm{e}^{-(\beta_V(\beta)/2)(\theta-2\pi n)^2}. \tag{4}$$

He then expanded both sides in a Fourier series

$$I_0(\beta) + 2\sum_{b=1}^{\infty} I_b(\beta)\cos b\theta \approx \frac{R_V(\beta)}{\sqrt{2\pi\beta_V(\beta)}}\left(1 + 2\sum_{b=1}^{\infty} \mathrm{e}^{-b^2/2\beta_V(\beta)}\cos b\theta\right) \tag{5}$$

and determined the unknown functions $R_V(\beta)$ and $\beta_V(\beta)$ by the requirement that the lowest Fourier coefficients for $b=0$ and $b=\pm 1$ be equal. This led to

$$R_V(\beta) = I_0(\beta)\sqrt{2\pi\beta_V}, \tag{6}$$

$$\mathrm{e}^{-1/2\beta_V(\beta)} = \frac{I_1(\beta)}{I_0(\beta)}. \tag{7}$$

In the limit $\beta \to \infty$, these relations become

$$R_V(\beta) \to \mathrm{e}^{\beta}\left(1 - \frac{1}{4\beta} - \cdots\right),$$

$$\beta_V(\beta) \to \beta - \tfrac{1}{2} - \cdots, \tag{8}$$

in agreement with (1), (2).

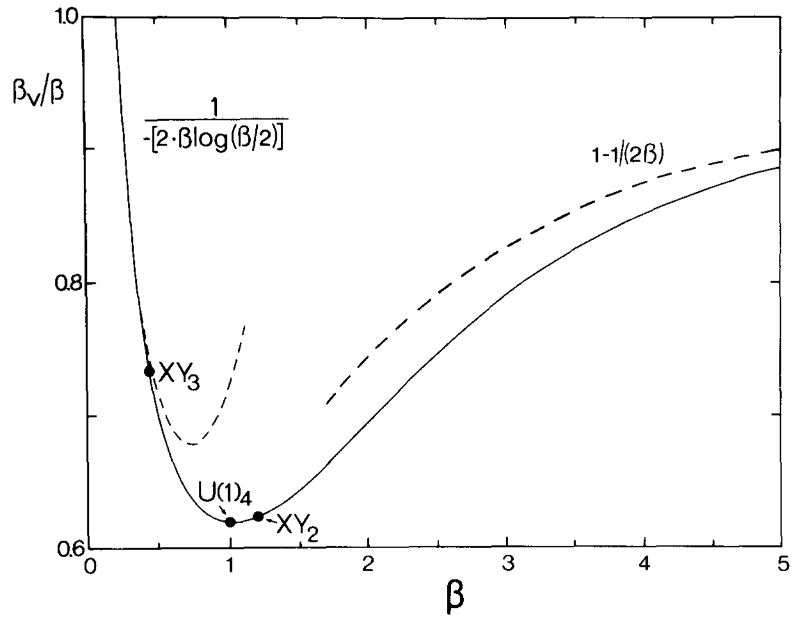

Fig. 1. The inverse temperature of the Villain approximation $\beta_V(\beta)$ as a function of β of the corresponding cosine model. The phase transitions are seen to lie in the low-β regime (for the $D = 3$ XY model, (9) is a good approximation).

In the opposite limit of small β they give

$$R_V(\beta) \sim \sqrt{2\pi\beta_V}\,,$$

$$\beta_V(\beta) \sim -[2\log(\beta/2)]^{-1}, \tag{9}$$

in agreement with (3).

In fig. 1, we have plotted β_V/β as a function of β and indicated the limiting forms (8), (9) by dashed lines. The high- and low-temperature regimes are clearly separated by the minimum of the curve which lies around $\beta \sim 1$. Notice that the limiting form at high temperatures, (9), approaches the full Villain approximation much faster than the low-temperature limit (8).

As a simple rough test of the quality of the approximation we may use the Monte Carlo data for the critical value β_c of the XY models and U(1) lattice gauge theory and compare them with the value β_{cVA} obtained from the critical value of the Villain model, β_{Vc}, via relation (7). The result is shown in table 1. We see that the agreement is excellent in all three cases. Notice that the three-dimensional XY critical point lies well inside the high-temperature regime, i.e. just opposite of the limit (1) usually invoked to introduce the Villain approximation. The critical points

TABLE 1
Comparison of critical temperature in XY model for $D = 2, 3$, and U(1) lattice gauge theory for $D = 4$ with the values obtained from the Villain approximation (VA) via $\beta_V = -[2\log(I_1(\beta)/I_0(\beta))]^{-1}$

Model	β_c	β_c (from VA)	β_{Vc}
2D-XY	1.12 [4a], 1.18 [4b]	1.18	0.73 [4c]
3D-XY	0.45 [4d]	0.45	0.33 [4e]
4D-U(1)	1.00 [4f]	1.02	0.63 [4g]

The values are taken from ref. [4], in which all but Ferer et al. (with results obtained from high-temperature series) obtained results from Monte Carlo simulation.

of the two-dimensional XY and the lattice gauge model, on the other hand, require the application of the full Villain formula (7) (see fig. 1).

The purpose of this paper is threefold: First we want to give a more detailed quantitative comparison of the three models with their Villain approximations. Second we want to clarify the physical content of the approximation. Third we show how the mapping cosine model ↔ Villain model can be made extremely precise (so that there are no differences in the order of the phase transition).

The partition functions we want to compare are

$$Z_{XY} = \prod_x \int \frac{d\theta(x)}{2\pi} \exp\left[\beta \sum_{x,i} \cos \nabla_i \theta(x)\right],$$

$$Z_{U(1)} = \prod_{x,i} \int \frac{d\theta_i(x)}{2\pi} \exp\left[\beta \sum_{x,i<j} \cos(\nabla_i \theta_j - \nabla_j \theta_i)\right] \tag{10}$$

and the Villain versions

$$Z_{XY}^{VM} = \prod_x \int \frac{d\theta(x)}{2\pi} \sum_{\{n_i(x)\}} \exp\left[-\tfrac{1}{2}\beta_V \sum_{x,i} (\nabla_i \theta - 2\pi n_i)^2\right],$$

$$Z_{U(1)}^{VM} = \prod_{x,i} \int \frac{d\theta_i(x)}{2\pi} \sum_{\{n_{ij}(x)\}} \exp\left[-\tfrac{1}{2}\beta_V \sum_{x,i<j} (\nabla_i \theta_j - \nabla_j \theta_i - 2\pi n_{ij})^2\right]. \tag{11}$$

Here x are the N sites of a D-dimensional simple cubic lattice, i the oriented links, and $\nabla_i \theta(x) \equiv \theta(x+i) - \theta(x)$ the lattice derivatives. Each of the partition functions has its own internal energy $u = -(1/N)(\partial/\partial\beta)\log Z$ and specific heat $c = -(\beta^2 \partial/\partial\beta)u$ with β replaced by β_V in the Villain case.

Using (4), the Villain approximation states that the partition functions should be related as follows

$$Z_{\mathrm{XY}} \approx R_{\mathrm{V}}(\beta)^{ND} Z_{\mathrm{XY}}^{\mathrm{VM}},$$
$$Z_{\mathrm{U(1)}} \approx R_{\mathrm{V}}(\beta)^{ND(D-1)/2} Z_{\mathrm{U(1)}}^{\mathrm{VM}}. \tag{12}$$

By forming the derivatives with respect to β, this leads to the following Villain approximation for the internal energy and specific heat

$$u_{\mathrm{XY}} \approx -D\frac{\dot{R}_{\mathrm{V}}}{R_{\mathrm{V}}} + \dot{\beta}_{\mathrm{V}} u_{\mathrm{XY}}^{\mathrm{VM}},$$
$$c_{\mathrm{XY}} \approx \beta^2\left[D\left(\frac{\ddot{R}_{\mathrm{V}}}{R_{\mathrm{V}}} - \frac{\dot{R}_{\mathrm{V}}^2}{R_{\mathrm{V}}^2}\right) - \ddot{\beta}_{\mathrm{V}} u_{\mathrm{XY}}^{\mathrm{VM}} + \frac{\dot{\beta}_{\mathrm{V}}^2}{\beta_{\mathrm{V}}^2} c_{\mathrm{XY}}^{\mathrm{VM}}\right], \tag{13}$$

with the same relations for the U(1) lattice gauge theory except that D has to be replaced by $\frac{1}{2}D(D-1)$ (i.e. the number of links by the number of plaquettes). The dots denote the derivatives with respect to β and give, explicitly

$$\dot{\beta}_{\mathrm{V}}(\beta) = -2\beta_{\mathrm{V}}^2\left(\mathrm{e}^{-1/2\beta_{\mathrm{V}}} - \mathrm{e}^{1/2\beta_{\mathrm{V}}} + \frac{1}{\beta}\right),$$
$$\dot{R}_{\mathrm{V}}(\beta) = R_{\mathrm{V}}\left(\mathrm{e}^{-1/2\beta_{\mathrm{V}}} + \tfrac{1}{2}\dot{\beta}_{\mathrm{V}}/\beta\right),$$
$$\ddot{\beta}_{\mathrm{V}}(\beta) = 2\dot{\beta}^2/\beta_{\mathrm{V}} + 2\beta_{\mathrm{V}}^2\left[\left(\mathrm{e}^{-1/\beta_{\mathrm{V}}} - \mathrm{e}^{1/\beta_{\mathrm{V}}}\right) + \frac{1}{\beta}\left(\mathrm{e}^{-1/2\beta_{\mathrm{V}}} + \mathrm{e}^{1/2\beta_{\mathrm{V}}}\right) + \frac{1}{\beta^2}\right],$$
$$\frac{\ddot{R}_{\mathrm{V}}(\beta)}{R_{\mathrm{V}}(\beta)} - \frac{\dot{R}_{\mathrm{V}}(\beta)^2}{R_{\mathrm{V}}(\beta)^2} = \frac{1}{2}\left[\frac{\ddot{\beta}_{\mathrm{V}}}{\beta_{\mathrm{V}}} - \frac{\dot{\beta}_{\mathrm{V}}^2}{\beta_{\mathrm{V}}^2}\right] + 1 - \frac{1}{\beta}\mathrm{e}^{-1/2\beta_{\mathrm{V}}} - \mathrm{e}^{-1/\beta_{\mathrm{V}}}. \tag{14}$$

In figs. 2–4 we have taken the Monte Carlo data for the internal energy and the specific heat of the Villain model, transformed them via (13), and plotted them on top of the Monte Carlo data of the corresponding cosine models*. The approximation is seen to be excellent for low β, up to the phase transition β_c. Above the transition it becomes rapidly worse. Around $\beta \approx 1.5$, the approximation produces an unphysical bump. Only for very high β does it reproduce the correct Dulong-Petit limits

$$u_{\mathrm{XY}} \to \frac{1}{2\beta},$$
$$c_{\mathrm{XY}} \to \frac{1}{2}. \tag{15}$$

* In all simulations, we have used cubic lattices with periodic boundary conditions, approximated the phase variables by 16 discrete angles $(2\pi/16)n$, $n = 0, \ldots, 15$, and worked with the heat-bath algorithm.

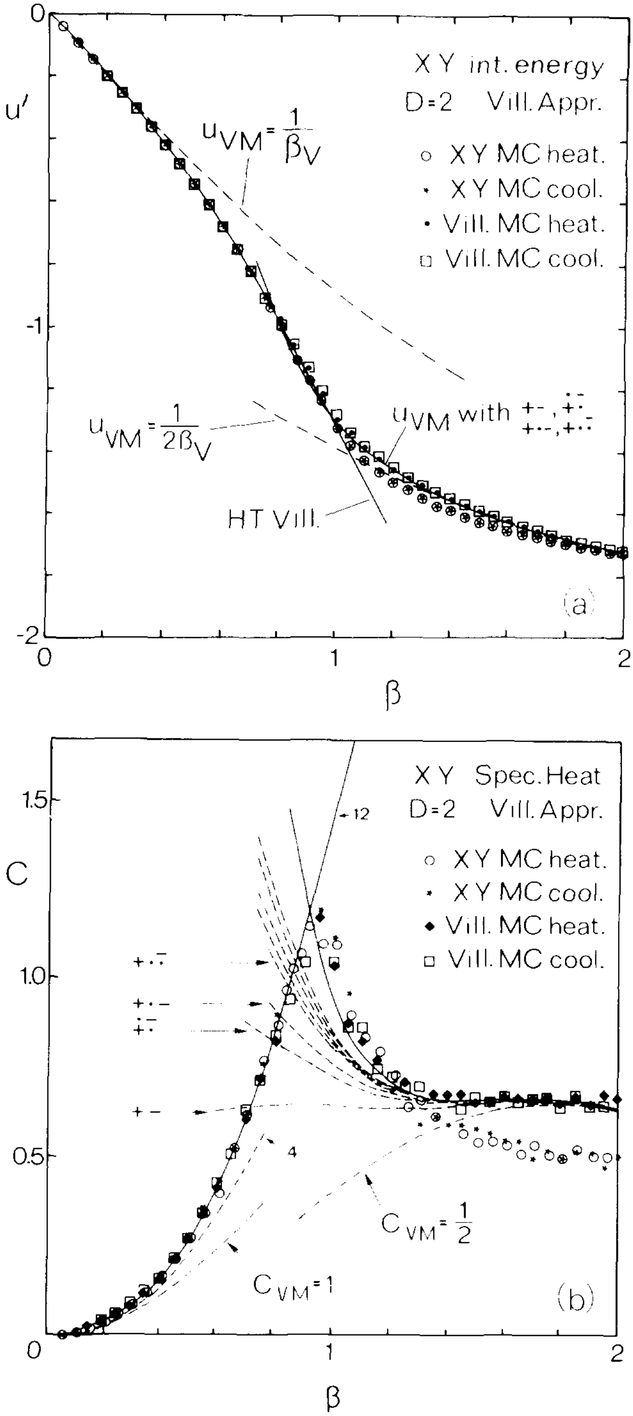

Fig. 2. The internal energy and the specific heat of the $D = 2$ XY model in comparison with the Villain approximation. The curves are obtained from high- and low-temperature expansions of the Villain model transformed in the same way.

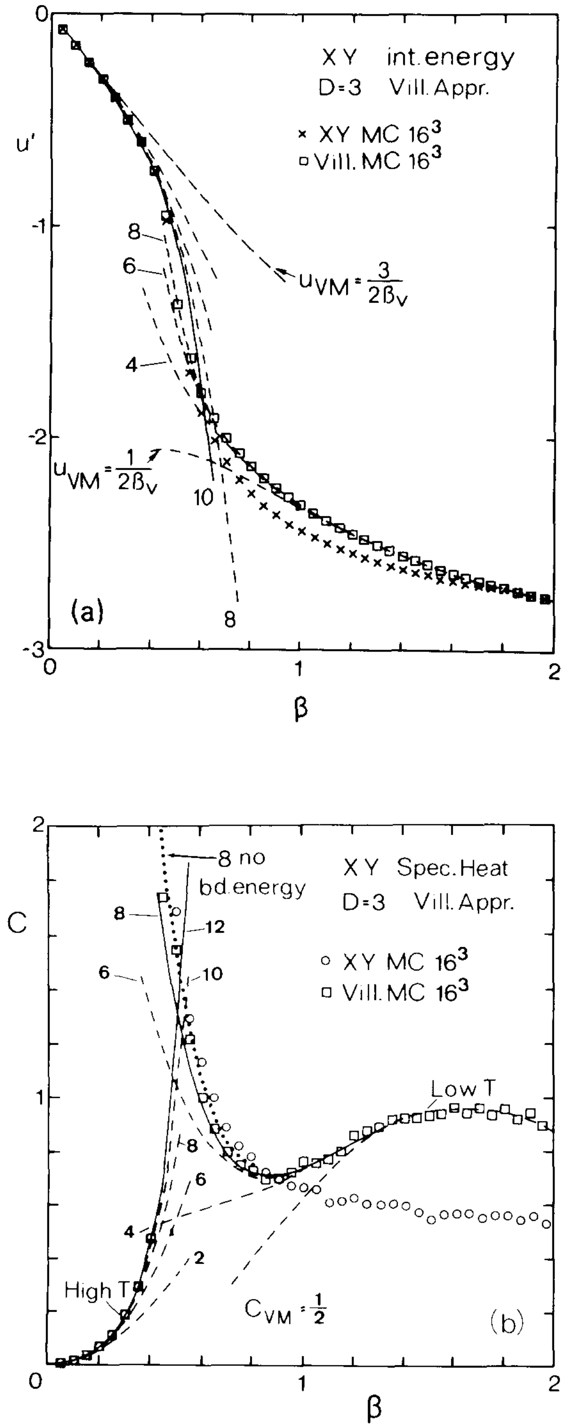

Fig. 3. The same comparison as in fig. 2 for $D = 3$ dimensions.

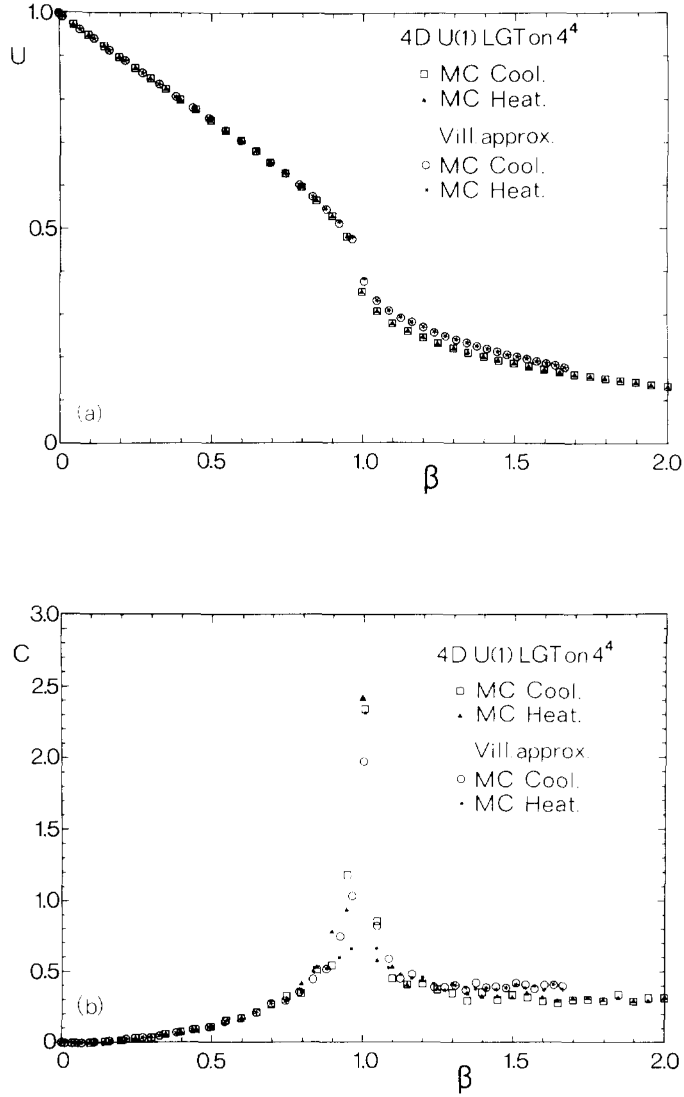

Fig. 4. The same comparison as in figs. 2, 3 for the $D = 4$ dimensional U(1) lattice gauge theory. In (c), (d), the critical regime is displayed with higher resolution and better statistics (500 and 2500 sweeps for equilibration and measurement, respectively). At first sight, the failure of the Villain approximation to the specific heat at $\beta \sim 1.5$ looks smaller than for the $D = 2$ XY model. This, however, is an optical illusion caused by the height of the peak (which the Kosterlitz-Thouless transition in the $D = 2$ XY model does not have). Percentage-wise, the deviation is the same.

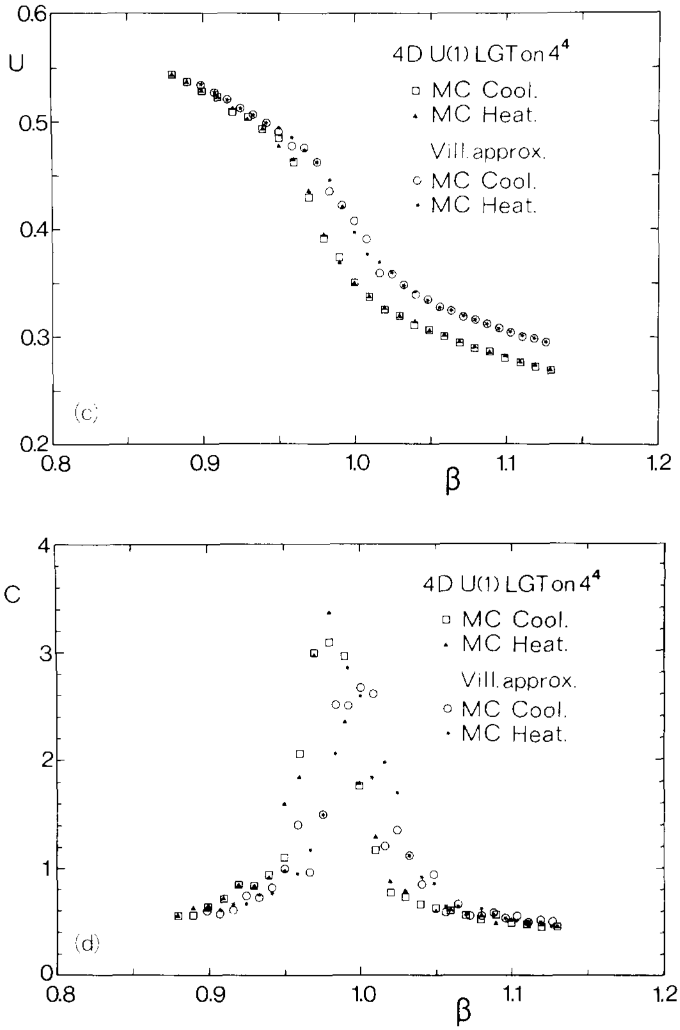

Fig. 4 continued.

In figs. 2 and 3 we have taken the high-and low-temperature expansions of the Villain model [5], transformed them via (13), and plotted them as well. The lowest dashed curve on the low-temperature side is due to the Dulong-Petit limit of the Villain model

$$u_{\rm XY}^{\rm VM} \sim \frac{1}{2\beta_{\rm V}},$$
$$c_{\rm XY}^{\rm VM} \sim \frac{1}{2}. \tag{16}$$

It fits very well into the unpleasant bumps.

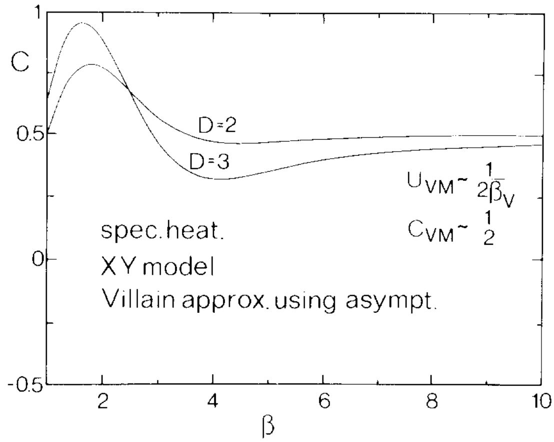

Fig. 5. The Villain approximation to the specific heat of the XY model for $D = 2, 3$ at large β using the large-β_V limits of the Villain model $u^{VM} \to 1/2\beta_V$, $c^{VM} \to \frac{1}{2}$. We see that very large $\beta \gtrsim 2.5$ are necessary to reach the correct limits.

In order to show the high values of β which are necessary for the Villain approximation to approach the correct Dulong-Petit limits we have plotted the Villain transformed limits (16) in fig. 5. Only for $\beta \geqslant 4$ does one reach the limits (15). In conclusion, the Villain approximation is a good low-β approximation, up to the phase transition. At moderately high β it is very bad and the limit (1), which is usually involved to justify its introduction, is reached so slowly that it is of no practical relevance.

Let us now come to our second task, namely that of understanding the physics of the Villain approximation. The high-temperature expansion of the three models is well-known

$$Z_{XY} = \sum_{\{b_i(x)\}} \prod_{x} \delta_{\overline{\nabla}_i b_i(x),0} \prod_{x,i} I_{b_i(x)}(\beta),$$

$$Z_{U(1)} = \sum_{\{f_{ij}(x)\}} \prod_{x,j} \delta_{\overline{\nabla}_i f_{ij}(x),0} \prod_{x,i<j} I_{f_{ij}(x)}(\beta). \tag{17}$$

The integer numbers $b_i(x)$ with the lattice divergence condition $\overline{\nabla}_i b_i(x) \equiv \Sigma_i (b_i(x) - b_i(x - i)) = 0$ describe closed non-self-backtracking lines of superflow [5]. Similarly, the integer numbers $f_{ij}(x)$, $i<j$ describe closed random surfaces [6]. For the Villain model, the equivalent expansion reads

$$Z_{XY}^{VM} = \frac{1}{(2\pi\beta_V)^{ND}} \sum_{\{b_i(x)\}} \prod_{x} \delta_{\overline{\nabla}_i b_i(x),0} \exp\left[-\sum_{x,i} \frac{b_i^2(x)}{2\beta_V} \right],$$

$$Z_{U(1)}^{VM} = \frac{1}{(2\pi\beta_V)^{ND(D-1)/2}} \sum_{\{f_{ij}(x)\}} \prod_{x,j} \delta_{\overline{\nabla}_i f_{ij}(x),0} \exp\left[-\sum_{x,i<j} \frac{f_{ij}^2(x)}{2\beta_V} \right]. \tag{18}$$

Comparison with (17) shows that the Villain approximation (12) with the relations (6), (7) would be *exact* if the sums were restricted to only the lowest values $b_i, f_{ij} = 0, \pm 1, \ldots$. The excellent quality of the approximation observed in figs. 2–4 teaches us that for low β, up to the phase transition, the systems are *dominated* by the lines or surfaces of strength one. Up to β_c, these lines or surfaces have a much larger entropy than the lines of larger strength and this is what gives them an overwhelming importance. The failure of the approximation *above* the transition must be due to lines and surfaces of strength larger than one.

The question arises whether the inclusion of lines and surfaces of strength two is capable of extending the validity of the approximation beyond the transition into the regime of moderate and large β. In order to see this we extend the Villain approximation (4) by writing an ansatz

$$e^{\beta\cos\theta + \gamma\cos 2\theta} \approx R_V^\gamma(\beta) \sum_n e^{-(\beta_V^\gamma/2)(\theta - 2\pi n)^2} \tag{19}$$

and asking for an *exact equality* of the lowest *three* Fourier coefficients. On the left-hand side, these are given by the generalized modified Bessel functions

$$I_b^\gamma(\beta) = \int_{-\pi}^{\pi} \frac{d\theta}{2\pi} \cos b\theta \, e^{\beta\cos\theta + \gamma\cos 2\theta} . \tag{20}$$

On the right-hand side, they are again

$$\frac{R_V^\gamma(\beta)}{\sqrt{2\pi\beta_V^\gamma}} e^{-b^2/2\beta_V^\gamma} .$$

Equating the terms $b = 0, \pm 1, \pm 2$ we find

$$R_V(\beta) = I_0^\gamma(\beta)\sqrt{2\pi\beta_V^\gamma} , \tag{21}$$

$$e^{-1/2\beta_V^\gamma(\beta)} = \frac{I_1^\gamma(\beta)}{I_0^\gamma(\beta)} , \tag{22}$$

$$e^{-4/2\beta_V^\gamma(\beta)} = \frac{I_2^\gamma(\beta)}{I_0^\gamma(\beta)} . \tag{23}$$

The solutions to the latter two equations are shown in fig. 6. When plotted in a β, γ plane, the Villain model runs along the curve given in fig. 7. For small β, the curve

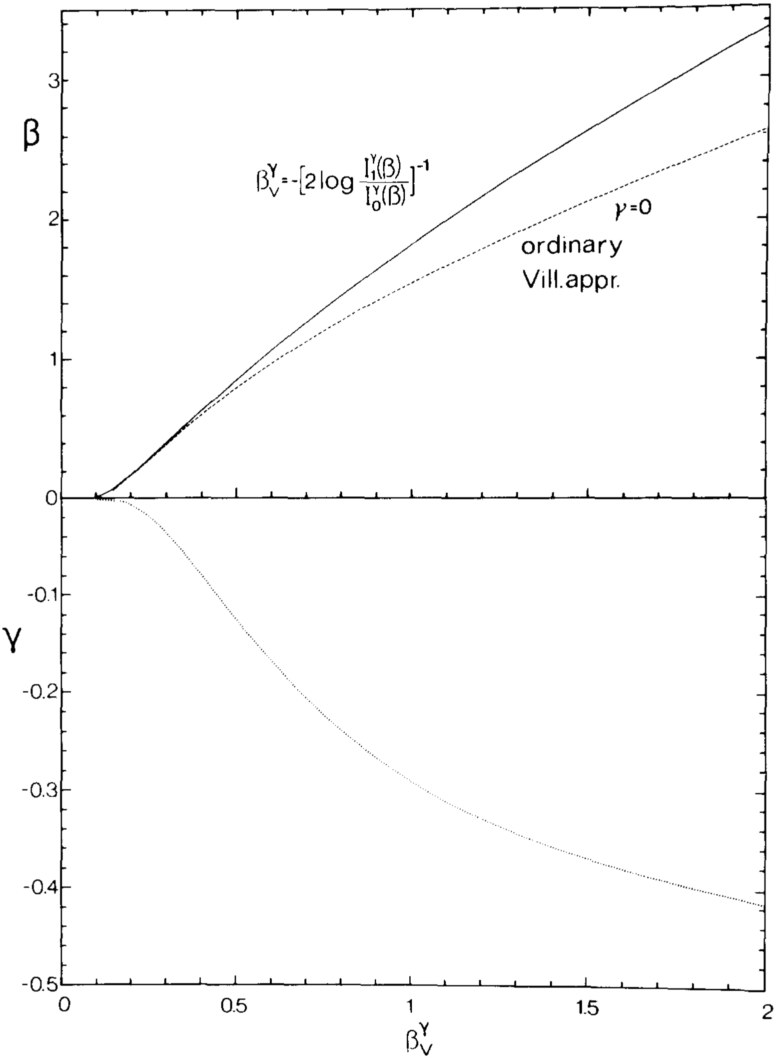

Fig. 6. The curves $\beta(\beta_V^\gamma)$ and $\gamma(\beta_V^\gamma)$ of the action $\beta \cos \theta + \gamma \cos 2\theta$ which is approximated best by the Villain model.

starts out with $\gamma \sim -\frac{1}{4}\beta^2$ and $\beta_V^\gamma \sim -[2\log(\beta/2)]^{-1}$. For large β, we find $\beta_V^\gamma \sim \beta + 4\gamma$ and $\gamma \sim -\frac{1}{16}\beta$ (see the appendix).

Let us test this improved Villain approximation by comparing the internal energy and specific heat of the U(1) gauge Villain model obtained by Monte Carlo simulations with the corresponding quantities obtained from the Monte Carlo data of the mixed cosine model, transformed via (19). Explicitly, if we denote $\nabla_i \theta_j(\boldsymbol{x}) - \nabla_j \theta_i(\boldsymbol{x})$ by θ_p with the label $p = (\boldsymbol{x}, i, j)$ for $i < j$ running through all plaquettes on

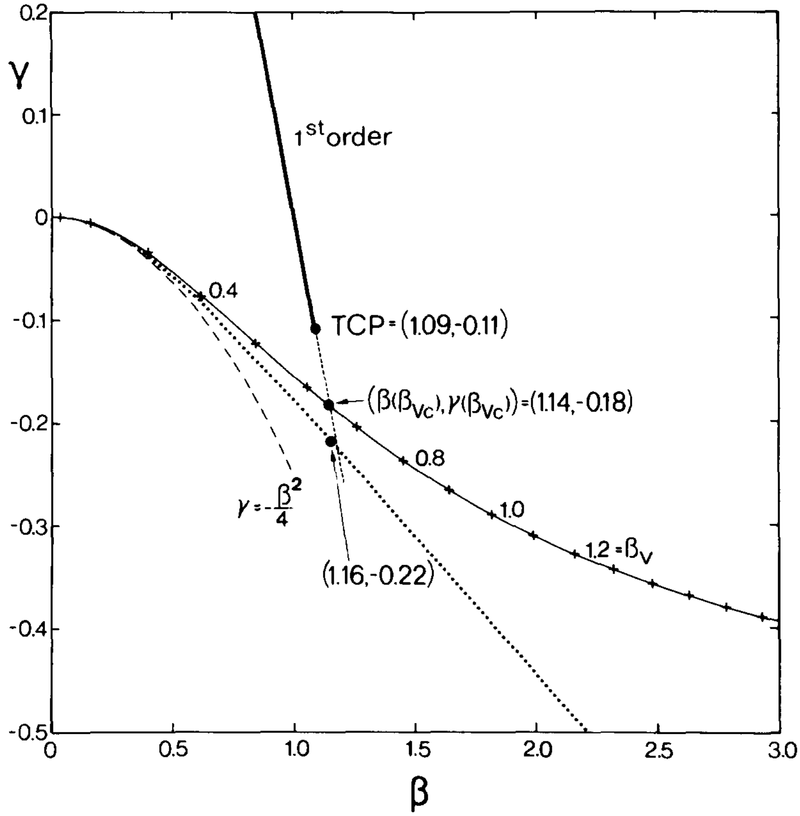

Fig. 7. The parameters β, γ of the mixed action $\beta\cos\theta + \gamma\cos 2\theta$ which can be studied by means of our improved Villain approximation. The fat vertical line shows a straight-line connection to the critical points found by Jersák et al. ([7]). The dotted line was estimated by those authors to be the locus of the Villain model in a different way from ours (which we believe to be less accurate).

the lattice, whose total number is $N_p = N\frac{1}{2}D(D-1)$, we determine the expectations and variances

$$c_n = \frac{1}{N_p}\sum_p \langle \cos n\theta_p \rangle ,$$

$$v_{nm} = N_p\left[\frac{1}{N_p^2}\sum_{p,p'}\langle \cos n\theta_p \cos m\theta_{p'}\rangle - c_n c_m\right] \tag{24}$$

in the model with the energy $\beta\Sigma_p\cos\theta_p + \gamma\Sigma_p\cos 2\theta_p$, and find from these the approximation to the internal energy and the specific heat of the Villain model as follows

$$u^{\mathrm{VM}} \approx \frac{1}{2\beta_{\mathrm{V}}} + \frac{\partial}{\partial\beta_{\mathrm{V}}}\log I_0^{\gamma}(\beta) - \frac{\partial\beta}{\partial\beta_{\mathrm{V}}}c_1 - \frac{\partial\gamma}{\partial\beta_{\mathrm{V}}}c_2,$$

$$c^{\mathrm{VM}} \approx \tfrac{1}{2} + \beta_{\mathrm{V}}^2\left[-\frac{\partial^2}{\partial\beta_{\mathrm{V}}^2}\log I_0^{\gamma}(\beta) + \frac{\partial^2\beta}{\partial\beta_{\mathrm{V}}^2}c_1 + \frac{\partial^2\gamma}{\partial\beta_{\mathrm{V}}^2}c_2 + \left(\frac{\partial\beta}{\partial\beta_{\mathrm{V}}}\right)^2 v_{11} + 2\frac{\partial\beta}{\partial\beta_{\mathrm{V}}}\frac{\partial\gamma}{\partial\beta_{\mathrm{V}}}v_{12} + \left(\frac{\partial\gamma}{\partial\beta_{\mathrm{V}}}\right)^2 v_{22}\right], \tag{25}$$

where we have omitted the superscript γ of β_{V} for brevity.

The results are plotted in fig. 8, together with the Monte Carlo data of the Villain model itself. The discrepancy above the phase transition, which is present in the ordinary Villain approximation, disappears completely. Near the critical point, both the internal energy and the specific heat are fitted perfectly.

The result is quite interesting in the light of the recent observation [7], suggested by one of the authors*, that the U(1) lattice gauge theory has a first-order transition. If we take the transition values [7] for the $\beta\cos\theta + \gamma\cos 2\theta$ model and insert them into our fig. 7, we see that they lie on a straight line with a tricritical point half-way between the pure cosine and the pure Villain model. In fig. 7, we also display another curve (the dotted one) which was suggested by Jersák et al. [7] to represent the locus of the Villain model in the β, γ plane. Those authors Fourier expanded the *logarithm* of the Villain-Boltzmann factor and truncated after the second term.

The pure cosine model has a transition entropy of about $\Delta s \approx 0.016$. When looking at fig. 8, we see that this is precisely the difference between the internal energies of the cosine and the mixed model above the transition. Since these models differ in the inclusion of the random surfaces of strength two we conclude that the transition entropy is carried almost entirely by these surfaces.

For completeness, we have compared the Boltzmann factor of the Villain model near the critical point with the corresponding $e^{\beta\cos\theta}$ and $e^{\beta\cos\theta+\gamma\cos 2\theta}$ expressions in fig. 9.

Finally, let us mention that due to the focus on the lower Fourier components, neither the ordinary Villain approximation nor our improvement of it can be used to calculate reliably expectations or correlations of cosines of multiple angles. This is illustrated in fig. 10.

* See ref. [8a]. The proof is based on a combination of the result of Coleman and Weinberg [8b] with the duality transformation of the U(1) lattice gauge theory to the abelian Higgs model of one of the authors [8c].

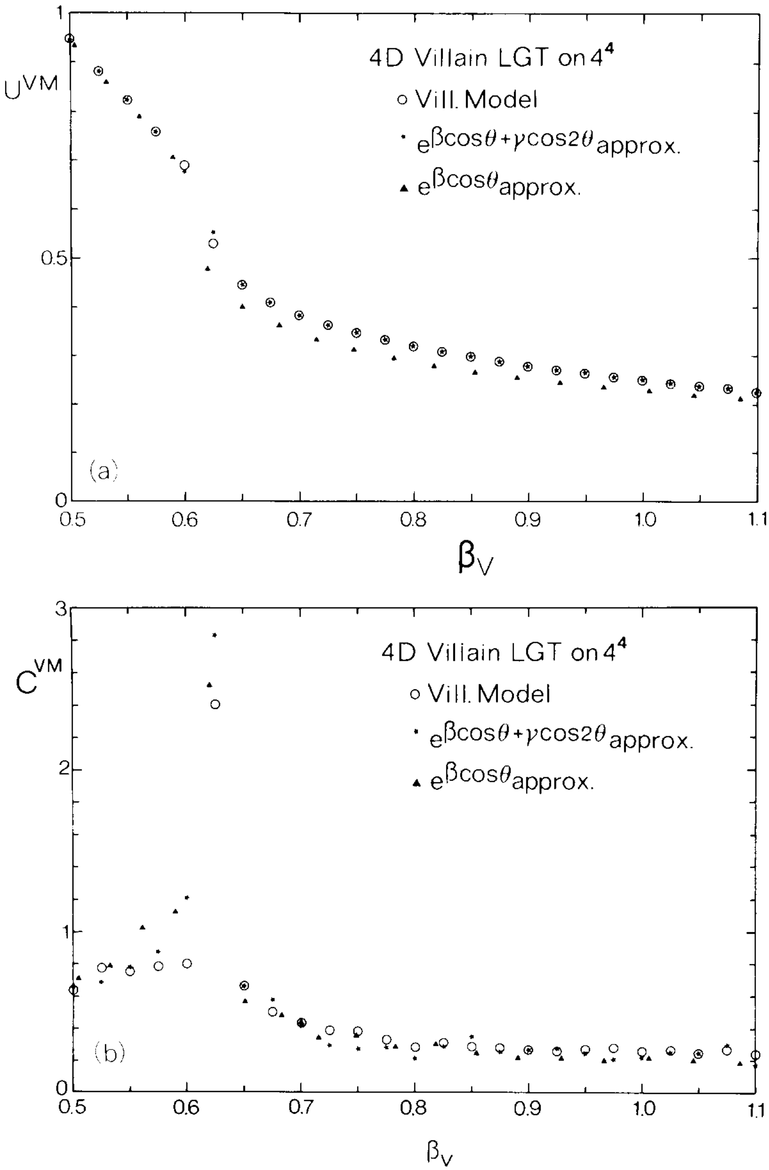

Fig. 8. The internal energy and the specific heat of the U(1) lattice gauge Villain model obtained on a 4^4 lattice with 150 and 750 sweeps for equilibration and measurement, respectively. The lower data points are obtained from Monte Carlo simulations of the $\beta \cos\theta$ model (on the same lattice) transformed according to the original Villain prescription. The stars which fall practically on top of the Villain data are from a simulation of a model with action $\cos\theta + \gamma\cos 2\theta$ treated according to our improved Villain approximation (19). The removal of the discrepancy is due to the inclusion of random surfaces of strength two in the high-temperature expansion.

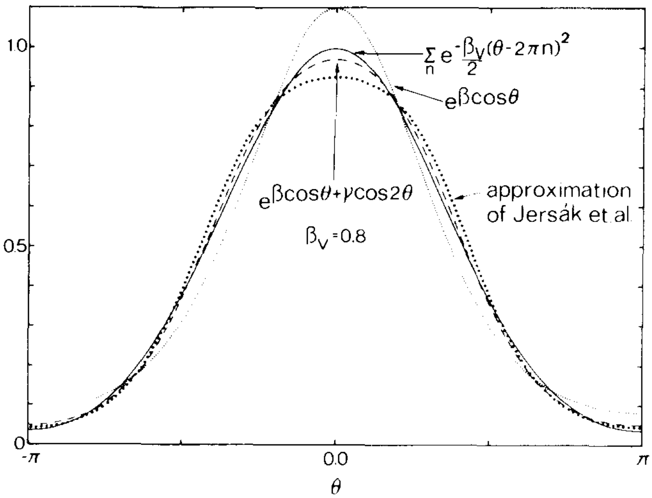

Fig. 9. Comparison of the Boltzmann factors of the three models of the U(1) lattice gauge theory at $\beta_V = 0.8$. Villain $\Sigma_n e^{(\beta_V/2)(\theta-2\pi n)^2}$ (—), $e^{\beta\cos\theta}$ (···), related via (4), $e^{\beta\cos\theta+\gamma\cos 2\theta}$ (---) related via (19), and $e^{\beta\cos\theta+\gamma\cos 2\theta}$ (●●●) related by Jersák et al., ref. [7].

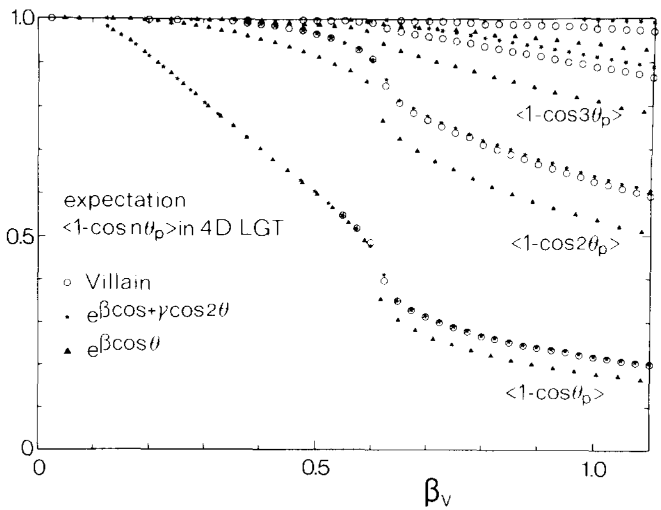

Fig. 10. The expectation of cosines of multiple angles in the Villain model as compared with the $\beta\cos\theta$ model, related via (4), or the $\beta\cos\theta + \gamma\cos 2\theta$ model, related via (19). For large multiples, the approximation becomes rapidly worse. The internal energy is mostly due to $\cos\theta$ and a little $\cos 2\theta$ and thus approximated very well.

Appendix

THE ASYMPTOTIC LIMIT $\beta \to \infty$

Assuming $\beta + 4\gamma > 0$, the integral

$$I_0^\gamma(\beta) = \int_{-\pi}^{\pi} \frac{d\theta}{2\pi} e^{\beta\cos\theta + \gamma\cos 2\theta} \tag{A.1}$$

has a maximum at $\theta = 0$. In the limit $\beta \to \infty$, $\gamma/\beta = \text{const} > -\frac{1}{4}$, we expand

$$I_0^\gamma(\beta) = e^{\beta+\gamma} \int_{-\pi}^{\pi} \frac{d\theta}{2\pi}$$
$$\times \exp\left[-\tfrac{1}{2}(\beta+4\gamma)\theta^2 + \tfrac{1}{24}(\beta+16\gamma)\theta^4 - \tfrac{1}{720}(\beta+64\gamma)\theta^6 + \cdots\right].$$

Changing variables to $\theta' \equiv \sqrt{\tfrac{1}{2}(\beta+4\gamma)}\,\theta$ we calculate

$$I_0^\gamma(\beta) = e^{\beta+\gamma}\sqrt{\frac{1}{2\pi(\beta+4\gamma)}} \int_{-\infty}^{\infty} \frac{d\theta}{\sqrt{\pi}} e^{-\theta^2}\left(1 + \frac{1}{6}\frac{\beta+16\gamma}{(\beta+4\gamma)^2}\theta^4\right.$$
$$\left. - \frac{1}{90}\frac{\beta+64\gamma}{(\beta+4\gamma)^3}\theta^6 + \frac{1}{2}\frac{1}{36}\frac{(\beta+16\gamma)^2}{(\beta+4\gamma)^4}\theta^8 + \cdots\right) \tag{A.2}$$

by using the integrals

$$\int_{-\infty}^{\infty} \frac{d\theta}{\sqrt{\pi}} e^{-\theta^2}\theta^{2n} = \frac{(2n-1)!!}{2^n}$$

and find the series

$$I_0^\gamma(\beta) = \frac{e^{\beta+\gamma}}{\sqrt{2\pi(\beta+4\gamma)}}\left(1 + \frac{3}{4\cdot 6}\frac{\beta+16\gamma}{(\beta+4\gamma)^2} - \frac{15}{8\cdot 90}\frac{\beta+64\gamma}{(\beta+4\gamma)^3}\right.$$
$$\left. + \frac{105}{2\cdot 36\cdot 16}\frac{(\beta+16\gamma)^2}{(\beta+4\gamma)^4} + \cdots\right). \tag{A.3}$$

This gives

$$\log I_0^\gamma(\beta) = \beta + \gamma - \tfrac{1}{2}\log[2\pi(\beta+4\gamma)] + \frac{1}{8}\frac{\beta+16\gamma}{(\beta+4\gamma)^2}$$
$$+ \frac{1}{16}\frac{\beta^2 + 20\beta\gamma + 16^2\gamma^2}{(\beta+4\gamma)^4} + \cdots. \tag{A.4}$$

From this we find

$$\frac{I_1^\gamma(\beta)}{I_0^\gamma(\beta)} = \frac{\partial}{\partial\beta}\log I_0^\gamma(\beta)$$

$$= 1 - \frac{1}{2(\beta+4\gamma)} - \frac{1}{8}\frac{\beta+28\gamma}{(\beta+4\gamma)^3} - \frac{\beta^2+26\beta\gamma+472\gamma^2}{8(\beta+4\gamma)^5} + \cdots, \tag{A.5}$$

$$\frac{I_2^\gamma(\beta)}{I_0^\gamma(\beta)} = \frac{\partial}{\partial\gamma}\log I_0^\gamma(\beta)$$

$$= 1 - \frac{2}{\beta+4\gamma} + \frac{\beta-8\gamma}{(\beta+4\gamma)^3} + \frac{1}{4}\frac{\beta^2+68\beta\gamma-512\gamma^2}{(\beta+4\gamma)^5} + \cdots. \tag{A.6}$$

We now impose the condition

$$\frac{I_2^\gamma(\beta)}{I_0^\gamma(\beta)} = \left(\frac{I_1^\gamma(\beta)}{I_0^\gamma(\beta)}\right)^4. \tag{A.7}$$

From (A.5), the right-hand side is equal to

$$1 - \frac{2}{\beta+4\gamma} + \frac{\beta-8\gamma}{(\beta+4\gamma)^3} - \frac{\beta^2-28\beta\gamma+640\gamma^2}{4(\beta+4\gamma)^5}. \tag{A.8}$$

Comparing this with (A.6), we see that only the last term brings in a possible difference between the two sides in (A.7). We can therefore determine γ from the quadratic equation

$$\gamma^2 + \tfrac{5}{16}\beta\gamma + \tfrac{1}{64}\beta^2 = 0, \tag{A.9}$$

or

$$\gamma_{\substack{1\\2}} = \begin{cases} -\tfrac{1}{4}\beta \\ -\tfrac{1}{16}\beta. \end{cases} \tag{A.10}$$

Only the second solution satisfies the condition $\gamma/\beta > -\frac{1}{4}$ and gives the correct answer (see the curve in fig. 7 which shows also the next term to be $\gamma \to -\frac{1}{16}\beta - 0.22 + O(1/\beta)$). From eq. (A.5) we read off directly

$$\beta_V \xrightarrow[\beta\to\infty]{} \beta + 4\gamma = \tfrac{3}{4}\beta + \cdots \tag{A.11}$$

and $\beta \to \frac{4}{3}\beta_V + 0.6$; $\gamma \to -\frac{1}{12}\beta_V - 0.26$ (see fig. 6 for the constants).

Finally, it is worth pointing out that the weak coupling expansion of the partition function of the mixed model can be obtained directly from eq. (A.2) by replacing

$$\theta^2 \to \sum_p \theta_p^2 \,.$$

It is then easy to see that on the Villain locus, $\gamma = -\frac{1}{16}\beta$-const, the leading corrections to the (gaussian) Dulong-Petit law are of order $1/\beta^2$, whereas for $\gamma = 0$ (Wilson model) they start out with the usual $1/\beta$ term.

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