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# Spin–spin correlation function in the high-temperature Villain model

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**Abstract.** We consider the spin–spin correlation function in the high-temperature regime of the generalised Villain model. Using the 'Debye–Huckel' approximation plus systematic corrections, we show that this correlation function has the expected Ornstein–Zernike form, and we calculate approximately the high-temperature behaviour of the correlation length. The methods presented here should prove useful in matching calculations of thermodynamic quantities in the two-dimensional $XY$ model, and in 'Debye–Huckel' analyses of a variety of two-dimensional Coulomb gas problems.

Much attention has been focused in recent years on the properties of the two-dimensional $XY$ model (for reviews, see Halperin 1979, Nelson 1980). This model exhibits no conventional long-range order (Hohenberg 1967, Mermin and Wagner 1966), yet it is believed to have two distinct thermodynamic phases, separated by a continuous phase transition (Kosterlitz and Thouless 1973, Kosterlitz 1974). In the low-temperature phase the system is populated by spin waves and tightly bound vortex pairs of equal and opposite vorticity, mostly of unit strength. The spin–spin correlation function in this phase decays algebraically. The vortex pairs begin to unbind above the Kosterlitz–Thouless transition and, at sufficiently high temperatures, all of the pairs are unbound and vortices of all strengths are present. One expects that in the latter regime, the spin–spin correlation function should have the Ornstein–Zernike (Ornstein and Zernike 1914) form appropriate for two dimensions, namely:

$$g(\boldsymbol{r}-\boldsymbol{r}') = \langle \exp[\mathrm{i}(\theta(\boldsymbol{r})-\theta(\boldsymbol{r}')]\rangle$$
$$\sim \exp(-\xi^{-1}|\boldsymbol{r}-\boldsymbol{r}'|)/(|\boldsymbol{r}-\boldsymbol{r}'|)^{1/2}, \qquad \text{as } |\boldsymbol{r}-\boldsymbol{r}'|\to\infty \tag{1}$$

where $\theta(\boldsymbol{r})$ is the spin polar angle.

In this paper we study $g(\boldsymbol{r}-\boldsymbol{r}')$ at high temperatures in the generalised Villain model (Villain 1975, José *et al* 1977) which is closely related to the $XY$ model. Swendsen (1978, see also Holz 1979) has shown previously that $g(\boldsymbol{r}-\boldsymbol{r}')$ decays *exponentially* in the high-temperature regimes of the Villain and $XY$ models using a general *roughening* representation, and has calculated the temperature dependence of $\xi$. Here we show that $g(\boldsymbol{r}-\boldsymbol{r}')$ has the full form (1) in the generalised Villain model using the 'Debye–Huckel' approximation plus systematic corrections (for a discussion of 'Debye–Huckel'

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theory in the context used here, see Berker and Nelson 1979, and Nelson and Halperin 1979). Our calculation, carried out in the *Coulomb gas* representation is useful for several reasons. First, the techniques presented here allow a 'Debye–Huckel' treatment of any of the two-dimensional Coulomb gas problems where two sets of charges interact via the function $\Phi(\boldsymbol{r}) = \tan^{-1}(y/x)$, $\boldsymbol{r} = (x, y)$. These problems include the Villain model in symmetry-breaking fields, the clock models (Elitzur *et al* 1979), the two-layer $XY$ model (Parga and Van Himbergen, 1980), and tilted hexatic phases (Nelson and Halperin 1980), (for further examples and general discussion, see Kadanoff 1978). Second, $g(\boldsymbol{r}-\boldsymbol{r}')$ and similar correlation functions in the $XY$ model can now be approximately calculated at *all* temperatures using the Nelson–Rudnick matching formalism (Rudnick and Nelson 1976, Nelson 1976). By means of the Kosterlitz (1974) recursion relations (which are phrased in the Coulomb gas language) $g(\boldsymbol{r}-\boldsymbol{r}')$ can be iterated away from the critical region to a temperature, say twice $T_c$ and then matched onto the result of our calculation. An analogous matching calculation for the specific heat has been carried out by Berker and Nelson (1979), and Solla and Riedel (1980). Finally, using methods similar to ours, Ostlund and Halperin (1980) have studied the behaviour of the displacement correlation function in the nematic-like phase above the melting temperature of anisotropic layers of molecules.

We begin our calculation with the expression for $g(\boldsymbol{r}-\boldsymbol{r}')$ derived by José *et al* (1977) in the generalised Villain model, namely:

$$g(\boldsymbol{r}-\boldsymbol{r}') = g_{\mathrm{sw}}(\boldsymbol{r}-\boldsymbol{r}')g_{\mathrm{v}}(\boldsymbol{r}-\boldsymbol{r}') \tag{2a}$$

where the spin-wave contribution is given by

$$g_{\mathrm{sw}}(\boldsymbol{r}-\boldsymbol{r}') = 1/|\boldsymbol{r}-\boldsymbol{r}'|^{\eta}, \qquad \eta = 1/2\pi K \tag{2b}$$

and the vortex correlation function is given by

$$g_{\mathrm{v}}(\boldsymbol{r}-\boldsymbol{r}') = \left\langle \exp \mathrm{i} \sum_{\boldsymbol{R}} m(\boldsymbol{R})u(\boldsymbol{R}) \right\rangle_{\mathrm{v}} \tag{2c}$$

for a collection of vortices $\{m(\boldsymbol{R})\}$ on sites $\boldsymbol{R}$ of the dual lattice. The expectation value $(2c)$ is calculated in the vortex ensemble given by the action,

$$A[m] = \sum_{\boldsymbol{R}} m^2(\boldsymbol{R}) \ln y + \sum_{\text{pairs}} 2\pi K m(\boldsymbol{R})m(\boldsymbol{R}') \ln |\boldsymbol{R}-\boldsymbol{R}'| \tag{3}$$

and the vortex partition function $Z_{\mathrm{v}}$ is the sum of $\exp\{A[m]\}$ over all vortex configurations. The function $u(\boldsymbol{R})$ appearing in $(2c)$ is given by

$$u(\boldsymbol{R}) = \Phi(\boldsymbol{r}-\boldsymbol{R}) - \Phi(\boldsymbol{r}'-\boldsymbol{R}). \tag{4}$$

The expression for $g(\boldsymbol{r}-\boldsymbol{r}')$ given by $(2a\text{–}c)$ can be understood intuitively by decomposing the spin polar angle $\theta(\boldsymbol{r})$ as follows:

$$\theta(\boldsymbol{r}) = \phi(\boldsymbol{r}) + \sum_{\boldsymbol{R}} m(\boldsymbol{R})\Phi(\boldsymbol{r}-\boldsymbol{R}) \tag{5}$$

where $\phi(\boldsymbol{r})$ represents the spin-wave degree of freedom and ranges over all real values, and the second term in (5) is the spin angle at site $\boldsymbol{r}$ due to a set of vortices $\{m(\boldsymbol{R})\}$ on the dual lattice. Inserting (5) into the definition (1) of $g(\boldsymbol{r}-\boldsymbol{r}')$, and noting that the spin-wave and vortex degrees of freedom decouple in the Villain model we arrive at the results $(2a\text{–}c)$ after integrating out the spin-wave degrees of freedom. The function

$u(\boldsymbol{R})$ can be interpreted as the difference in spin angles at sites $\boldsymbol{r}$ and $\boldsymbol{r}'$ due to a unit vortex at the dual lattice site $\boldsymbol{R}$.

José *et al* (1977) have constructed a low-temperature expansion of the vortex correlation function (2*c*), valid when the vortex pairs are tightly bound. We consider the opposite limit, namely the high-temperature regime where the pairs are unbound and vortices of all strengths are present. To construct a systematic high-temperature expansion we utilise the Poisson sum formula which states:

$$\sum_{m=-\infty}^{+\infty} g(m) = \sum_{p=-\infty}^{+\infty} \int_{-\infty}^{+\infty} \mathrm{d}\phi g(\phi) \exp(-2\pi \mathrm{i} p\phi) \tag{6}$$

for any function $g$. Thus, we can rewrite (2*c*) as follows:

$$g_{\mathrm{v}}(\boldsymbol{r}-\boldsymbol{r}') = Z_{\mathrm{v}}^{-1} \sum_{\{m(\boldsymbol{R})\}} \exp\left\{\mathrm{i} \sum_{\boldsymbol{R}} m(\boldsymbol{R}) u(\boldsymbol{R}) + A[m]\right\}$$

$$= \frac{\Sigma_{\{p(\boldsymbol{R})\}} \Pi_{\boldsymbol{R}} \int_{-\infty}^{+\infty} \mathrm{d}\phi(\boldsymbol{R}) \exp(A[\phi] + \mathrm{i}\,\Sigma_{\boldsymbol{R}} (2\pi p(\boldsymbol{R}) + u(\boldsymbol{R}))\phi(\boldsymbol{R}))}{\Sigma_{\{p(\boldsymbol{R})\}} \Pi_{\boldsymbol{R}} \int_{-\infty}^{+\infty} \mathrm{d}\phi(\boldsymbol{R}) \exp(A[\phi])}. \tag{7}$$

Integrating (7) over the fields $\phi(\boldsymbol{R})$ we obtain

$$g_{\mathrm{v}}(\boldsymbol{r}-\boldsymbol{r}') = Z'/Z \tag{8a}$$

where

$$Z' = \sum_{\{p(\boldsymbol{R})\}} \exp\left(-\frac{1}{2} \sum_{\boldsymbol{R},\boldsymbol{R}'} (u(\boldsymbol{R}) + 2\pi p(\boldsymbol{R})) G(\boldsymbol{R}-\boldsymbol{R}')(u(\boldsymbol{R}') + 2\pi p(\boldsymbol{R}'))\right) \tag{8b}$$

and

$$Z = \sum_{\{p(\boldsymbol{R})\}} \exp\left(-\frac{1}{2} \sum_{\boldsymbol{R},\boldsymbol{R}'} 2\pi p(\boldsymbol{R}) G(\boldsymbol{R}-\boldsymbol{R}') 2\pi p(\boldsymbol{R}')\right). \tag{8c}$$

The Green function $G(\boldsymbol{R}-\boldsymbol{R}')$ is a short-ranged interaction given by

$$G(\boldsymbol{R}) = \langle m(0) m(\boldsymbol{R})\rangle_{\mathrm{DH}}$$

$$= \int \mathrm{d}^2 q \frac{1-\exp(\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{R})}{4\pi^2 K - 8\pi q^2 (\ln y + \pi^2 K/2)}. \tag{9}$$

The expectation value $\langle m(0)m(\boldsymbol{R})\rangle_{\mathrm{DH}}$ is the charge–charge correlation function evaluated in the 'Debye–Huckel' approximation (Berker and Nelson 1979, and Nelson and Halperin 1979), i.e., setting $\{p(\boldsymbol{R}) = 0\}$ and thereby replacing sums over the discrete charges $\{m(\boldsymbol{R})\}$ by integrals over the continuous fields $\{\phi(\boldsymbol{R})\}$. For simplicity we take $G(\boldsymbol{R})$ to be a nearest-neighbour interaction. The functions $Z$ and $Z'$ (8*b*, *c*) can then be rewritten as follows:

$$Z' = \sum_{\{p(\boldsymbol{R})\}} \exp\left(-\frac{1}{16\pi^2 K} \sum_{\langle \boldsymbol{R},\boldsymbol{R}'\rangle} (u(\boldsymbol{R}) + 2\pi p(\boldsymbol{R}) - u(\boldsymbol{R}') - 2\pi p(\boldsymbol{R}'))^2\right) \tag{10a}$$

$$Z = \sum_{\{p(\boldsymbol{R})\}} \exp\left(-\frac{1}{16\pi^2 K} \sum_{\langle \boldsymbol{R},\boldsymbol{R}'\rangle} (2\pi p(\boldsymbol{R}) - 2\pi p(\boldsymbol{R}'))^2\right) \tag{10b}$$

where we have used the overall charge neutrality condition in the form

$$\sum_{\boldsymbol{R}} \langle m(0) m(\boldsymbol{R})\rangle_{\mathrm{DH}} = 0. \tag{11}$$

A systematic high-temperature (small $K$) expansion for $g_v(\boldsymbol{r}-\boldsymbol{r}')$ can now be developed by considering excitations in the integer field $\{p(\boldsymbol{R})\}$. Some configurations with $p(\boldsymbol{R})\neq 0$ contribute to the long-distance behaviour of $g_v(\boldsymbol{r}-\boldsymbol{r}')$ with the same weight as the configuration $\{p(\boldsymbol{R})=0\}$ and thus, unlike the evaluation of $Z_v$ (Berker and Nelson 1979), systematic corrections to the 'Debye–Hückel' approximation must be taken into account here. First, it is convenient to note an alternative interpretation of $u(\boldsymbol{R})$, namely: $u(\boldsymbol{R})$ is the spin angle at site $\boldsymbol{R}$ due to a positive unit vortex at $\boldsymbol{r}$ and a negative unit vortex at $\boldsymbol{r}'$. To arrange that $u(\boldsymbol{R})$ will be a single-valued function, we introduce a cut running from $\boldsymbol{r}$ to $\boldsymbol{r}'$. For simplicity we choose $\boldsymbol{r}$ and $\boldsymbol{r}'$ to lie on the same horizontal row, and choose the cut to be the shortest path between the two points (see figure 1). The angle $u(\boldsymbol{R})$ decreases by $2\pi$ as we cross the cut from below. The configurations of the integer field $\{p(\boldsymbol{R})\}$ and their contributions to $Z$ and $Z'$ can best be enumerated graphically. We note that at sufficiently high temperatures only values of $|p(\boldsymbol{R})|\leq 1$ need be considered, and we represent $(u(\boldsymbol{R})+2\pi p(\boldsymbol{R})-u(\boldsymbol{R}')-2\pi p(\boldsymbol{R}'))^2$ or $(2\pi p(\boldsymbol{R})-2\pi p(\boldsymbol{R}'))^2$ as bonds bisecting the line joining $\boldsymbol{R}$ and $\boldsymbol{R}'$ if their values are $4\pi^2$. Our graphical conventions are illustrated in figures 1–3. Note that certain configurations of $\{p(\boldsymbol{R})\}$ will effectively shift the position of the cut; thus our original choice for the cut is irrelevant, as we will ultimately sum over all paths joining $\boldsymbol{r}$ and $\boldsymbol{r}'$. The absence of a bond in the graphs for $Z'$ denotes that $u(\boldsymbol{R})+2\pi p(\boldsymbol{R})$ varies

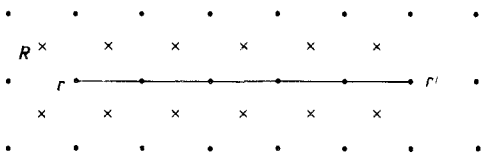


**Figure 1.** The $\{p(\boldsymbol{R})=0\}$ contribution to $Z'$. The full circles represent lattice sites populated by the spin polar angle field $\theta(\boldsymbol{r})$, while the crosses denote sites of the dual lattice $\boldsymbol{R}$, populated by the integer field $\{p(\boldsymbol{R})\}$. This graph represents our choice for the cut joining $\boldsymbol{r}$ and $\boldsymbol{r}'$. When nearest-neighbour sites $\boldsymbol{R}$ and $\boldsymbol{R}'$ are on opposite sides of the cut, $(u(\boldsymbol{R})-u(\boldsymbol{R}'))^2=4\pi^2$.

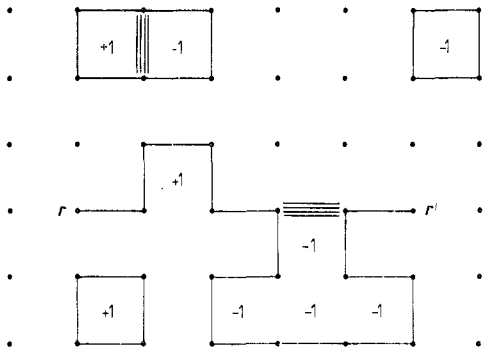


**Figure 2.** An example of a graph contributing to $Z'$ when some $p(\boldsymbol{R})\neq 0$. A bond on the lattice represents $(u(\boldsymbol{R})+2\pi p(\boldsymbol{R})-u(\boldsymbol{R})-2\pi p(\boldsymbol{R}'))^2=4\pi^2$ where $\boldsymbol{R}$ and $\boldsymbol{R}'$ are nearest-neighbour sites on opposite sides of the bond. Non-zero values of $p(\boldsymbol{R})$ are shown as numbers on dual lattice sites; the absence of a number indicates $p(\boldsymbol{R})=0$. Polygons separated from the chain joining $\boldsymbol{r}$ and $\boldsymbol{r}'$ are invariant under $p\rightarrow -p$. However, excitations of $p(\boldsymbol{R})$ which form the chain do not satisfy this invariance. Deleting the chain between $\boldsymbol{r}$ and $\boldsymbol{r}'$ would yield a graph for $Z$.

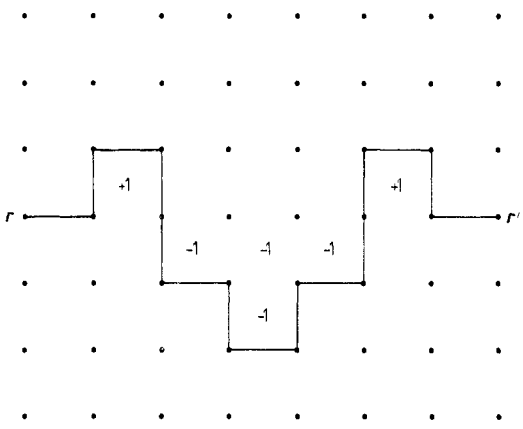


**Figure 3.** An example of the type of graph considered in the 'no-overhang' approximation (14) for $g_v$.

continuously from $R$ to $R'$, and we can replace $(u(\boldsymbol{R})+2\pi p(\boldsymbol{R})-u(\boldsymbol{R}')-2\pi p(\boldsymbol{R}'))^2$ by $(\nabla_R u(\boldsymbol{R}))^2$. The absence of a bond in the graphs for $Z$ contributes zero to the argument of the exponential in (10*b*). In general, the graphical expansions of $Z$ and $Z'$ are quite complex. The function $Z$ is the sum over all closed polygons with up to four bonds on a side in some cases, and each graph is weighted by the appropriate power of $e^{-1/K}$. The function $Z'$ is the sum over all self-avoiding open chains from $\boldsymbol{r}$ to $\boldsymbol{r}'$ and closed polygons which can intersect and share bonds with the chain (see figure 2). Each graph in the series for $Z'$ will be multiplied by the appropriate power of $e^{-1/K}$ and by the factor,

$$\exp\left\{\frac{1}{8\pi^2 K}\int' (\nabla_R u(\boldsymbol{R}))^2 \,\mathrm{d}^2R\right\} \tag{12}$$

where the primed integral denotes an integration over all space with the exception of the lines of the graph. The integration over $(\nabla_R u)^2$ can be done by parts,

$$\int' (\nabla_R u(\boldsymbol{R}))^2 \,\mathrm{d}^2R = -\int' u(\boldsymbol{R})\nabla_R^2 u(\boldsymbol{R})\,\mathrm{d}^2R + \int_G u(\boldsymbol{R})\nabla_R u(\boldsymbol{R})\cdot \mathrm{d}\boldsymbol{\sigma} \tag{13}$$

where $\mathrm{d}\boldsymbol{\sigma}$ is the normal to the graph lines. The first integral on the right-hand side of (13) vanishes since $\nabla_R^2 u = 0$. The second integral is taken (a) on a closed contour at infinity, where it vanishes, and (b) along both sides of the graph lines, in opposite senses. The path integrals along the interior and exterior of closed polygons separated from the self-avoiding chain mutually cancel (see figure 4). Then, upon dividing $Z'$ by $Z$, the polygonal counting factors in both functions which are proportional to $N^x$, $x \geqslant 1$ (where $N$ is the number of sites in the lattice) mutually cancel. To establish the Ornstein–Zernike form (1) we will neglect all of the remaining polygons, since the self-avoiding configurations should dominate numerically. Furthermore, we will consider only self-avoiding walks with no overhangs. This approximation should be reasonable at high temperatures. The vortex correlation function can now be written as,

$$g_v(\boldsymbol{r}-\boldsymbol{r}') = \sum_n P_n(\boldsymbol{r}-\boldsymbol{r}')\exp(-n/4k)\exp\left\{\frac{1}{8\pi^2 K}\int_G u(\boldsymbol{R})\nabla_R u(\boldsymbol{R})\cdot \mathrm{d}\boldsymbol{\sigma}\right\} \tag{14}$$

where $P_n(\boldsymbol{r}-\boldsymbol{r}')$ is the number of self-avoiding walks of length $n$ joining $\boldsymbol{r}$ and $\boldsymbol{r}'$ which

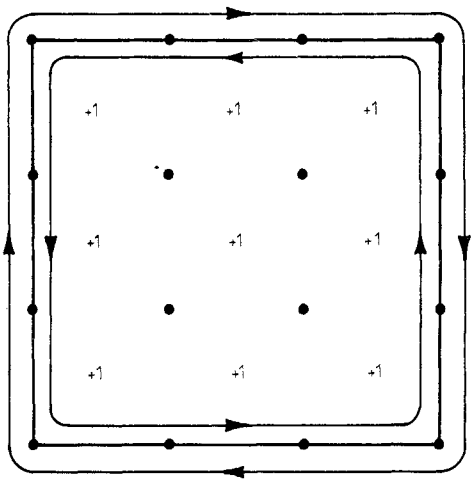


**Figure 4.** Illustration of the directions of path integrals around a typical polygon. The function $u(\boldsymbol{R})+2\pi p(\boldsymbol{R})$ along the interior path is equal to that function along the exterior path plus $2\pi$. Using $\nabla_R^2 u = 0$ it can be shown that the two path integrals mutually cancel.

do not have overhangs. The path integration in the second exponential factor in (14) yields,

$$\int_G u(\boldsymbol{R})\nabla_R u(\boldsymbol{R}) \cdot \mathrm{d}\boldsymbol{\sigma} = 4\pi \ln|r-r'|. \tag{15}$$

The calculation leading to (15) is identical to the evaluation of the interaction energy of a vortex–antivortex pair in the $XY$ model (see, e.g., de Gennes 1974). Thus, the factor

$$\exp\left\{\frac{1}{8\pi^2 K}\int_G u(\boldsymbol{R})\nabla_R u(\boldsymbol{R}) \cdot \mathrm{d}\boldsymbol{\sigma}\right\} = \exp(\eta \ln|r-r'|) \tag{16}$$

precisely cancels the spin-wave correlation function (2b). To complete the evaluation of $g_v(\boldsymbol{r}-\boldsymbol{r}')$, we sum over the weighted self-avoiding walks in (14) using a generating function (see, e.g., Domb 1954, Montroll and Weiss 1965):

$$\begin{aligned} g(\boldsymbol{r}-\boldsymbol{r}') &= \sum_n P_n(\boldsymbol{r}-\boldsymbol{r}')\exp(-n/4K) \\ &= \oint \frac{\mathrm{d}z}{z}\left(\mathrm{e}^{-1/4K} + \mathrm{e}^{-1/2K}z + \mathrm{e}^{-1/2K}z^{-1}\right)^{|r-r'|} \\ &= \int_{-\pi}^{\pi} \mathrm{d}\theta \exp\left(-\frac{1}{4K}|\boldsymbol{r}-\boldsymbol{r}'|\right)(1+2\mathrm{e}^{-1/4K}\cos\theta)^{|r-r'|}. \end{aligned} \tag{17}$$

At high temperatures we can approximate the above expression by,

$$\begin{aligned} g(\boldsymbol{r}-\boldsymbol{r}') &\approx \int_{-\pi}^{\pi} \mathrm{d}\theta \exp\left(-|\boldsymbol{r}-\boldsymbol{r}'|\left(\frac{1}{4K} - 2\,\mathrm{e}^{-1/4K}\cos\theta\right)\right) \\ &= \exp(-(1/4K)|\boldsymbol{r}-\boldsymbol{r}'|)I_0(2|\boldsymbol{r}-\boldsymbol{r}'|\,\mathrm{e}^{-1/4K}) \\ &\sim \exp\left[-\left(\frac{1}{4K} - 2\,\mathrm{e}^{-1/4K}\right)|\boldsymbol{r}-\boldsymbol{r}'|\right] \Big/ (|\boldsymbol{r}-\boldsymbol{r}'|)^{1/2} \qquad \text{as } |\boldsymbol{r}-\boldsymbol{r}'| \to \infty. \end{aligned} \tag{18}$$

Thus, we attain the Ornstein–Zernike form (1) with

$$\xi^{-1} = 1/4K - 2\,\mathrm{e}^{-1/4K} \tag{19}$$

which agrees with Swendsen's (1978) calculation to first order in $\mathrm{e}^{-1/4K}$. A more complete evaluation of $g_v(\boldsymbol{r}-\boldsymbol{r}')$ would presumably yield the full functional dependence of $\varepsilon^{-1}$ on $K$.

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