S8.A. Critical Exponents for the S^4 Model

Mathematical details concerning the Fourier series / transform can be found in §Appendix, where equations are labelled as (A.1), (A.2), ...

Consider a d-D cubic Ising lattice N lattice sites. The partition function can be written as

$$Z(K) = \sum_{\{S_m\}} \exp\left(\frac{1}{2} K \sum_{\boldsymbol{n}} \sum_{\boldsymbol{e}} S_{\boldsymbol{n}} S_{\boldsymbol{n}+\boldsymbol{e}} \right) \qquad S_{\boldsymbol{n}} = \pm 1 \tag{8.98}$$

where $K = \beta J$ and $\boldsymbol{e}$ is a vector pointing to a nearest neighbor of site $\boldsymbol{n}$.

For a cubic lattice with lattice constant a, the primitive lattice vectors are

$$\boldsymbol{a}_i = a\, \hat{\boldsymbol{x}}_i i = 1, \ \ldots, \ d \tag{8.98a}$$

where $\hat{\boldsymbol{x}}_i$ is the unit vector along the x_i-axis.

The site label $\boldsymbol{n}$ is a d-tuple of integers

$$\boldsymbol{n} = (n_1, \ \ldots, \ n_d) \qquad n_i = -M, \ \ldots, \ M-1 \tag{8.98b}$$

where M is an integer satisfying $(2\,M)^d = N$.

The spatial position of site $\boldsymbol{n}$ is therefore

$$\boldsymbol{x} = \sum_{i=1}^{d} n_i\, \boldsymbol{a}_i = \sum_{i=1}^{d} n_i\, a\, \hat{\boldsymbol{x}}_i = \boldsymbol{n}\, a \tag{8.98c}$$

Let $\mathbf{e}_i$ be the d-tuple of integers whose only non-zero component, of value 1, is at the i^{th} position, e.g.,

$$\mathbf{e}_1 = (1, 0, 0, \ \ldots) \qquad \mathbf{e}_2 = (0, 1, 0, \ \ldots)$$

The nearest neighbor labels are then given by

$$\mathbf{e}_i \text{ and } -\mathbf{e}_i \qquad i = 1, \ \ldots, \ d \tag{8.98d}$$

so that

$$\sum_{\boldsymbol{e}} S_{\boldsymbol{n}} S_{\boldsymbol{n}+\boldsymbol{e}} = S_{\boldsymbol{n}} S_{\boldsymbol{n}+\mathbf{e}_1} + \ldots + S_{\boldsymbol{n}} S_{\boldsymbol{n}+\mathbf{e}_d} + S_{\boldsymbol{n}} S_{\boldsymbol{n}-\mathbf{e}_1} + \ldots + S_{\boldsymbol{n}} S_{\boldsymbol{n}-\mathbf{e}_d} \tag{8.98e}$$

The factor $\frac{1}{2}$ in (8.98) is required since $\sum_{\boldsymbol{n}} \sum_{\boldsymbol{e}}$ counts each pair of interaction twice, i.e., $S_{\boldsymbol{n}} S_{\boldsymbol{n}+\mathbf{e}_i}$ and $S_{\boldsymbol{n}+\mathbf{e}_i} S_{(\boldsymbol{n}+\mathbf{e}_i)-\mathbf{e}_i} = S_{\boldsymbol{n}+\mathbf{e}_i} S_{\boldsymbol{n}}$ describe the same pair.

The summation

$$\sum_{\{S_m\}} \equiv \sum_{S_1=\pm 1} \cdots \sum_{S_N=\pm 1}$$

includes all possible spin configurations of the lattice. We can change it to an integral by means of a weighting factor

$$W(S_{\boldsymbol{n}}) = \delta\,(S_{\boldsymbol{n}} + 1) + \delta(S_{\boldsymbol{n}} - 1) = 2\,\delta\!\left(S_{\boldsymbol{n}}^2 - 1\right) \tag{8.99a}$$

so that

$$Z(K) = \prod_{\boldsymbol{m}} \int_{-\infty}^{\infty} d\, S_{\boldsymbol{m}}\, W(S_{\boldsymbol{m}}) \exp\left(\frac{1}{2} K \sum_{\boldsymbol{n}} \sum_{\boldsymbol{e}} S_{\boldsymbol{n}} S_{\boldsymbol{n}+\boldsymbol{e}} \right) \tag{8.99}$$

Note: It is common practice to write (8.99) as

$$Z(K) = \prod_{n} \int_{-\infty}^{\infty} d\, S_n\, W(S_n) \exp\left(\frac{1}{2} K \sum_{n} \sum_{e} S_n\, S_{n+e} \right)$$

It is advantageous to replace (8.98a) with a mathematically more manageable continuum version

$$W(S_n) = c \exp\left(-\frac{1}{2} b\, S_n^2 - u\, S_n^4 \right) \qquad (8.100)$$

where

$$c = \frac{1}{2} \pi e^{b^2/32\, u} \sqrt{\left| \frac{b}{u} \right|} \left[I_{-1/4}\left(\frac{b^2}{32\, u} \right) + I_{1/4}\left(\frac{b^2}{32\, u} \right) \right] \qquad (8.100a)$$

is a normalization constant and $I_n(z)$ is the modified Bessel function of the 1st kind [see "graphs.nb"].

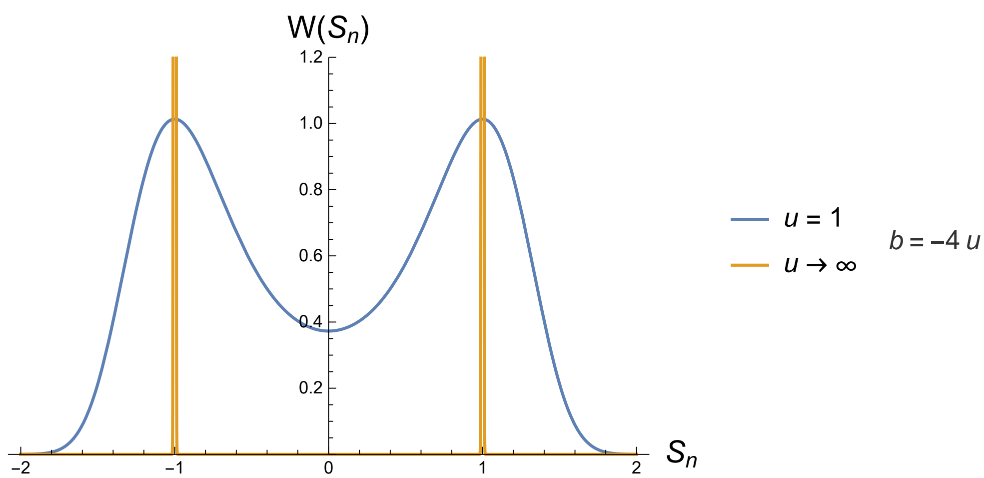
Following Reichl, we shall drop the normalization constant c since it will be cancelled out in any calculation of averages.

Setting $b = -4\, u$, (8.100) becomes

$$\begin{aligned} W(S_n) &= c \exp\left[-u \left(-2\, S_n^2 + S_n^4 \right) \right] \\ &= c\, e^u \exp\left[-u \left(S_n^2 - 1 \right)^2 \right] \\ &\to \exp\left[-u \left(S_n^2 - 1 \right)^2 \right] \end{aligned} \qquad (8.101)$$

where we've dropped the constant prefactor in the last expression.

Plot for the normalized $W(S_n)$ is shown below [see "graphs.nb"].



Using (8.100) on (8.99) gives

$$Z(K) = \prod_{m} \int_{-\infty}^{\infty} d\, S_m \exp\left[\frac{1}{2} K \sum_{n} \sum_{e} S_n\, S_{n+e} - \sum_{n} \left(\frac{1}{2} b\, S_n^2 + u\, S_n^4 \right) \right] \qquad (8.102)$$

This may be interpreted as a system with a Hamiltonian

$$\begin{aligned} \beta H &= -\frac{1}{2} K \sum_{n} \sum_{e} S_n\, S_{n+e} + \sum_{n} \left(\frac{1}{2} b\, S_n^2 + u\, S_n^4 \right) \\ &= -K \sum_{n} \sum_{e}{}' S_n\, S_{n+e} + \sum_{n} \left(\frac{1}{2} b\, S_n^2 + u\, S_n^4 \right) \end{aligned} \qquad (8.103a)$$

where [see (8.98a)]

$$\sum_{\boldsymbol{e}}{}' S_{\boldsymbol{n}} S_{\boldsymbol{n}+\boldsymbol{e}} \equiv \sum_{i=1}^{d} S_{\boldsymbol{n}} S_{\boldsymbol{n}+\boldsymbol{e}_i}$$

is a sum over only $\boldsymbol{e}$ in the "positive" direction.

Using

$$\sum_{\boldsymbol{n}}\sum_{\boldsymbol{e}}{}' S_{\boldsymbol{n}}^2 = d \sum_{\boldsymbol{n}} S_{\boldsymbol{n}}^2$$

$$\sum_{\boldsymbol{n}}\sum_{\boldsymbol{e}}{}' S_{\boldsymbol{n}+\boldsymbol{e}}^2 = \sum_{\boldsymbol{e}}{}' \sum_{\boldsymbol{n}-\boldsymbol{e}} S_{\boldsymbol{n}}^2 = \sum_{\boldsymbol{e}}{}' \sum_{\boldsymbol{n}} S_{\boldsymbol{n}}^2 \qquad \text{[Boundary terms neglected.]}$$

$$= d \sum_{\boldsymbol{n}} S_{\boldsymbol{n}}^2$$

$$\rightarrow \qquad \sum_{\boldsymbol{n}}\sum_{\boldsymbol{e}}{}' (S_{\boldsymbol{n}} - S_{\boldsymbol{n}+\boldsymbol{e}})^2 = -2 \sum_{\boldsymbol{n}}\sum_{\boldsymbol{e}}{}' S_{\boldsymbol{n}} S_{\boldsymbol{n}+\boldsymbol{e}} + 2\, d \sum_{\boldsymbol{n}} S_{\boldsymbol{n}}^2$$

we can write (8.103a) as

$$\beta H = \frac{1}{2} K \sum_{\boldsymbol{n}}\sum_{\boldsymbol{e}}{}' (S_{\boldsymbol{n}} - S_{\boldsymbol{n}+\boldsymbol{e}})^2 + \frac{1}{2} K \left(\frac{b}{K} - 2\, d\right) \sum_{\boldsymbol{n}} S_{\boldsymbol{n}}^2 + u \sum_{\boldsymbol{n}} S_{\boldsymbol{n}}^4 \qquad (8.103)$$

which is known as the S^4 Ising model.

Assuming periodic boundary conditions [see (A.6)], we can expand $S_{\boldsymbol{n}}$ as a Fourier series

$$S_{\boldsymbol{n}} = \frac{1}{N} \sum_{\boldsymbol{k} \in \mathrm{BZ}} S_{\boldsymbol{k}}\, e^{i \boldsymbol{k} \cdot \boldsymbol{n} a} \qquad (A.10)$$

together with its inverse

$$S_{\boldsymbol{k}} = \sum_{\boldsymbol{n}} S_{\boldsymbol{n}}\, e^{-i \boldsymbol{k} \cdot \boldsymbol{n} a} \qquad (A.12)$$

We have called the region

$$-\frac{\pi}{a} \le k_i < \frac{\pi}{a} \qquad i = 1, \ \ldots, d \qquad (A.8)$$

the Brillouin zone (BZ).

Comments:

1. $S_{\boldsymbol{n}}$ and $S_{\boldsymbol{k}}$ have the same dimensions (both are dimensionless).
2. Since $S_{\boldsymbol{k}}$ is only a mathematical construct to help describe the physical quantity $S_{\boldsymbol{n}}$, the constant prefactors in the Fourier series can be changed arbitrarily, with the difference absorbed in a re-defined $S_{\boldsymbol{k}}$. The difference between Reichl's (8.104) and (A.10) is therefore immaterial.

The following identity

$$\int_{\mathrm{BZ}} d\boldsymbol{k}\, e^{i \boldsymbol{k} \cdot \boldsymbol{n} a} = \left(\frac{2\pi}{a}\right)^d \prod_{i=1}^{d} \delta_{n_i 0} = \left(\frac{2\pi}{a}\right)^d \delta_{\boldsymbol{n} 0} \qquad (8.105)$$

is proved as (A.13) and the integration over the Brillouin zone is defined as

$$\int_{\mathrm{BZ}} d\boldsymbol{k} = \prod_{i=1}^{d} \int_{-\pi/a}^{\pi/a} d k_i \qquad (A.14)$$

Similarly,

$$\sum_{\boldsymbol{n}} e^{-i \boldsymbol{k} \cdot \boldsymbol{n} a} = \left(\frac{2\pi}{a}\right)^d \delta(\boldsymbol{k}) \qquad (8.106)$$

is proved as (A.17).

We can use (A.14) to write (A.10) as

$$S_{\boldsymbol{n}} = \left(\frac{2\pi}{a}\right)^d \int_{\mathrm{BZ}} d\boldsymbol{k}\, S_{\boldsymbol{k}}\, e^{i\boldsymbol{k}\cdot\boldsymbol{n}a}$$

Setting

$$\boldsymbol{x} = \boldsymbol{n}\,a \qquad\qquad S(\boldsymbol{k}) = S_{\boldsymbol{k}}$$

then gives

$$S(\boldsymbol{x}) = \left(\frac{2\pi}{a}\right)^d \int_{\mathrm{BZ}} d\boldsymbol{k}\, e^{i\boldsymbol{k}\cdot\boldsymbol{x}}\, S(\boldsymbol{k}) \tag{8.107}$$

$S(\boldsymbol{x})$ is therefore the continuum approximation of $S_{\boldsymbol{n}}$. Note that $S(\boldsymbol{x})$ & $S(\boldsymbol{k})$ are both dimensionless.

The next task is to get the continuum version of the Hamiltonian (8.103).

To begin, we use (8.104a) to write the 1st term as

$$\begin{aligned}
&\sum_{\boldsymbol{n}}\sum_{\boldsymbol{e}}{}' (S_{\boldsymbol{n}} - S_{\boldsymbol{n}+\boldsymbol{e}})^2 \\
&= \frac{1}{N^2}\sum_{\boldsymbol{n}}\sum_{\boldsymbol{e}}{}' \sum_{\boldsymbol{k},\boldsymbol{k}'\in\mathrm{BZ}} S_{\boldsymbol{k}}\left(e^{i\boldsymbol{k}\cdot\boldsymbol{n}a} - e^{i\boldsymbol{k}\cdot(\boldsymbol{n}+\boldsymbol{e})a}\right) S_{\boldsymbol{k}'}\left(e^{i\boldsymbol{k}'\cdot\boldsymbol{n}a} - e^{i\boldsymbol{k}'\cdot(\boldsymbol{n}+\boldsymbol{e})a}\right) \\
&= \frac{1}{N^2}\sum_{\boldsymbol{k},\boldsymbol{k}'\in\mathrm{BZ}} S_{\boldsymbol{k}} S_{\boldsymbol{k}'} \sum_{\boldsymbol{n}} e^{i(\boldsymbol{k}+\boldsymbol{k}')\cdot\boldsymbol{n}a} \sum_{\boldsymbol{e}}{}' \left(1 + e^{i(\boldsymbol{k}+\boldsymbol{k}')\cdot\boldsymbol{e}a} - e^{i\boldsymbol{k}'\cdot\boldsymbol{e}a} - e^{i\boldsymbol{k}\cdot\boldsymbol{e}a}\right) \\
&= \frac{1}{N}\sum_{\boldsymbol{k},\boldsymbol{k}'\in\mathrm{BZ}} S_{\boldsymbol{k}} S_{\boldsymbol{k}'}\, \delta_{\boldsymbol{k},-\boldsymbol{k}'} \sum_{\boldsymbol{e}}{}' \left(1 + e^{i(\boldsymbol{k}+\boldsymbol{k}')\cdot\boldsymbol{e}a} - e^{i\boldsymbol{k}'\cdot\boldsymbol{e}a} - e^{i\boldsymbol{k}\cdot\boldsymbol{e}a}\right) \\
&= \frac{1}{N}\sum_{\boldsymbol{k}\in\mathrm{BZ}} S_{\boldsymbol{k}} S_{-\boldsymbol{k}} \sum_{\boldsymbol{e}}{}' \left(2 - e^{-i\boldsymbol{k}\cdot\boldsymbol{e}a} - e^{i\boldsymbol{k}\cdot\boldsymbol{e}a}\right) \\
&= \frac{1}{N}\sum_{\boldsymbol{k}\in\mathrm{BZ}} S_{\boldsymbol{k}} S_{-\boldsymbol{k}} \sum_{\boldsymbol{e}}{}' \left|1 - e^{i\boldsymbol{k}\cdot\boldsymbol{e}a}\right|^2 \\
&= \left(\frac{a}{2\pi}\right)^d \int_{\mathrm{BZ}} d\boldsymbol{k}\, S(\boldsymbol{k})\, S(-\boldsymbol{k}) \sum_{\boldsymbol{e}}{}' \left|1 - e^{i\boldsymbol{k}\cdot\boldsymbol{e}a}\right|^2
\end{aligned} \tag{8.108}$$

Similarly, we get for the 2nd term,

$$\begin{aligned}
\sum_{\boldsymbol{n}} S_{\boldsymbol{n}}^2 &= \sum_{\boldsymbol{n}}\sum_{\boldsymbol{k},\boldsymbol{k}'\in\mathrm{BZ}} S_{\boldsymbol{k}} S_{\boldsymbol{k}'}\, e^{i(\boldsymbol{k}+\boldsymbol{k}')\cdot\boldsymbol{n}a} \\
&= \frac{1}{N}\sum_{\boldsymbol{k}\in\mathrm{BZ}} S_{\boldsymbol{k}} S_{-\boldsymbol{k}} \\
&= \left(\frac{a}{2\pi}\right)^d \int_{\mathrm{BZ}} d\boldsymbol{k}\, S(\boldsymbol{k})\, S(-\boldsymbol{k})
\end{aligned} \tag{8.108a}$$

And the 3rd term,

$$\begin{aligned}
\sum_{\boldsymbol{n}} S_{\boldsymbol{n}}^4 &= \sum_{\boldsymbol{n}}\sum_{\boldsymbol{k}_1,\boldsymbol{k}_2,\boldsymbol{k}_3,\boldsymbol{k}_4\in\mathrm{BZ}} S_{\boldsymbol{k}_1} S_{\boldsymbol{k}_2} S_{\boldsymbol{k}_3} S_{\boldsymbol{k}_4}\, e^{i(\boldsymbol{k}_1+\boldsymbol{k}_2+\boldsymbol{k}_3+\boldsymbol{k}_4)\cdot\boldsymbol{n}a} \\
&= \frac{1}{N^3}\sum_{\boldsymbol{k}_1,\boldsymbol{k}_2,\boldsymbol{k}_3,\boldsymbol{k}_4\in\mathrm{BZ}} S_{\boldsymbol{k}_1} S_{\boldsymbol{k}_2} S_{\boldsymbol{k}_3} S_{\boldsymbol{k}_4}\, \delta_{\boldsymbol{k}_1+\boldsymbol{k}_2+\boldsymbol{k}_3+\boldsymbol{k}_4,0} \\
&= \left(\frac{a}{2\pi}\right)^{3d} \int_{\mathrm{BZ}} d\boldsymbol{k}_1 \int_{\mathrm{BZ}} d\boldsymbol{k}_2 \int_{\mathrm{BZ}} d\boldsymbol{k}_3 \int_{\mathrm{BZ}} d\boldsymbol{k}_4 \\
&\qquad \times S(\boldsymbol{k}_1)\, S(\boldsymbol{k}_2)\, S(\boldsymbol{k}_3)\, S(\boldsymbol{k}_4)\, \delta(\boldsymbol{k}_1+\boldsymbol{k}_2+\boldsymbol{k}_3+\boldsymbol{k}_4)
\end{aligned} \tag{8.109}$$

(8.103) thus becomes

$$\beta H = \frac{1}{2} K \left(\frac{a}{2\pi} \right)^d \int_{BZ} d\,\boldsymbol{k}\, S(\boldsymbol{k})\, S(-\boldsymbol{k}) \sum_{\boldsymbol{e}}{}' \left| 1 - e^{i\,\boldsymbol{k}\cdot\boldsymbol{e}\,a} \right|^2 \tag{8.110}$$

$$+\left(\frac{1}{2} b - d\,K\right)\left(\frac{a}{2\pi} \right)^d \int_{BZ} d\,\boldsymbol{k}\, S(\boldsymbol{k})\, S(-\boldsymbol{k})$$

$$+u\left(\frac{a}{2\pi} \right)^{3d} \int_{BZ} d\,\boldsymbol{k}_1 \int_{BZ} d\,\boldsymbol{k}_2 \int_{BZ} d\,\boldsymbol{k}_3 \int_{BZ} d\,\boldsymbol{k}_4$$

$$\times S(\boldsymbol{k}_1)\, S(\boldsymbol{k}_2)\, S(\boldsymbol{k}_3)\, S(\boldsymbol{k}_4)\, \delta(\boldsymbol{k}_1 + \boldsymbol{k}_2 + \boldsymbol{k}_3 + \boldsymbol{k}_4)$$

Since $S_{\boldsymbol{n}}$ is real, (8.104a) gives

$$\sum_{\boldsymbol{k}} S_{\boldsymbol{k}}^* e^{-i\,\boldsymbol{k}\cdot\boldsymbol{n}\,a} = \sum_{\boldsymbol{k}} S_{\boldsymbol{k}}\, e^{i\,\boldsymbol{k}\cdot\boldsymbol{n}\,a} = \sum_{\boldsymbol{k}} S_{-\boldsymbol{k}}\, e^{-i\,\boldsymbol{k}\cdot\boldsymbol{n}\,a}$$

$$\rightarrow \qquad S_{\boldsymbol{k}}^* = S_{-\boldsymbol{k}} \qquad \rightarrow \qquad S^*(\boldsymbol{k}) = S(-\boldsymbol{k}) \tag{8.110a}$$

Near the critical point, long range order set in so that long wavelength ($k \to 0$) components dominate. Thus,

$$\sum_{\boldsymbol{e}}{}' \left| 1 - e^{i\,\boldsymbol{k}\cdot\boldsymbol{e}\,a} \right|^2 \approx \sum_{i=1}^{d} \left| \boldsymbol{k}\cdot\boldsymbol{e}_i\, a \right|^2 = \sum_{i=1}^{d} k_i^2\, a^2 = k^2\, a^2 \tag{8.110b}$$

(8.110) becomes

$$\beta H \approx \frac{1}{2} K\, a^2 \left(\frac{a}{2\pi} \right)^d \int_{BZ} d\,\boldsymbol{k} \left[k^2 + \frac{1}{a^2}\left(\frac{b}{K} - 2\,d \right) \right] \left| S(\boldsymbol{k}) \right|^2 \tag{8.111}$$

$$+u\left(\frac{a}{2\pi} \right)^{3d} \int_{BZ} d\,\boldsymbol{k}_1 \int_{BZ} d\,\boldsymbol{k}_2 \int_{BZ} d\,\boldsymbol{k}_3 \int_{BZ} d\,\boldsymbol{k}_4$$

$$\times S(\boldsymbol{k}_1)\, S(\boldsymbol{k}_2)\, S(\boldsymbol{k}_3)\, S(\boldsymbol{k}_4)\, \delta(\boldsymbol{k}_1 + \boldsymbol{k}_2 + \boldsymbol{k}_3 + \boldsymbol{k}_4)$$

We can absorb the $K\,a^2$ factor into the spin field by setting

$$S'(\boldsymbol{k}) = \sqrt{K\,a^2}\; S(\boldsymbol{k})$$

(8.111) then becomes

$$\beta H\left(r, u', \{S'\}\right) \approx \frac{1}{2} \left(\frac{a}{2\pi} \right)^d \int_{BZ} d\,\boldsymbol{k} \left(k^2 + r \right) \left| S'(\boldsymbol{k}) \right|^2 \tag{8.113}$$

$$+u'\left(\frac{a}{2\pi} \right)^{3d} \int_{BZ} d\,\boldsymbol{k}_1 \int_{BZ} d\,\boldsymbol{k}_2 \int_{BZ} d\,\boldsymbol{k}_3 \int_{BZ} d\,\boldsymbol{k}_4$$

$$\times S'(\boldsymbol{k}_1)\, S'(\boldsymbol{k}_2)\, S'(\boldsymbol{k}_3)\, S'(\boldsymbol{k}_4)\, \delta(\boldsymbol{k}_1 + \boldsymbol{k}_2 + \boldsymbol{k}_3 + \boldsymbol{k}_4)$$

where

$$r = \frac{1}{a^2}\left(\frac{b}{K} - 2\,d \right) \qquad\qquad u' = \frac{u}{\left(K\,a^2\right)^2} \tag{8.113a}$$

The corresponding partition function

$$Z(r, u') = \prod_{\boldsymbol{k}} \int d\,S'(\boldsymbol{k})\, e^{-\beta H(r, u', \{S'\})}$$

$$\equiv \int \mathcal{D}\, S'(\boldsymbol{k})\, e^{-\beta H(r, u', \{S'\})} \tag{8.114}$$

is a path (or functional) integral over all possible (complex) values of $S'(\boldsymbol{k})$.

(8.111) is the starting point of the renormalization theory for the S^4 model. Setting $u = 0$ gives the Gaussian model.

Following the procedure used in Ex. 8.1, we proceed to find the block Hamiltonian. To begin, we approximate the BZ with a d-ball of the same volume. The radius $\frac{\pi}{a'}$ of the d-ball is therefore given by [see (A.23)]

$$\frac{\pi^{d/2}}{\Gamma\left(\frac{d}{2}+1\right)}\left(\frac{\pi}{a'}\right)^d = \left(\frac{2\pi}{a}\right)^d \tag{8.114a}$$

Next, we introduce a scaling parameter $L > 1$ so that the BZ is separated into two regions,

$$R_{\mathfrak{S}} = \left\{ \boldsymbol{k} \;\middle|\; 0 \le k < \frac{\pi}{L\,a'} \right\} = \text{long wavelength region} \tag{8.114b}$$

$$R_{\sigma} = \left\{ \boldsymbol{k} \;\middle|\; \frac{\pi}{L\,a'} \le k < \frac{\pi}{a'} \right\} = \text{short wavelength region} \tag{8.114c}$$

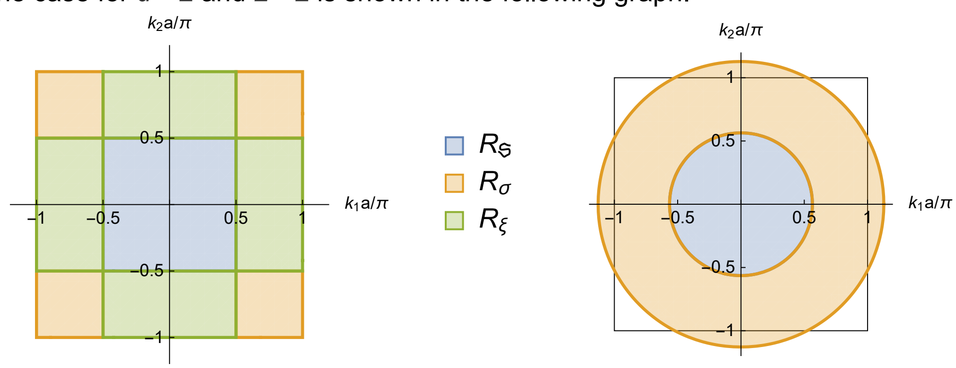
In contrast, the division scheme

$$R_{\mathfrak{S}} = \left\{ \boldsymbol{k} \;\middle|\; 0 < k_i < \frac{\pi}{L\,a} \;\; \forall\, i \right\}$$

$$R_{\sigma} = \left\{ \boldsymbol{k} \;\middle|\; \frac{\pi}{L\,a} < k_i < \frac{\pi}{a} \;\; \forall\, i \right\}$$

used by Reichl leaves out the region R_ξ composed of $\boldsymbol{k}$ points containing both short and long wavelength components. Its mathematical implementation is also more involved since the short wavelength region consists of disjointed parts. Finally, it contradicts with the usual interpretation that $e^{i\,\boldsymbol{k}\cdot\boldsymbol{x}}$ describes a plane wave of wave length $\lambda = \frac{2\pi}{k}$ traveling in the direction of $\boldsymbol{k}$.

The case for $d = 2$ and $L = 2$ is shown in the following graph.



Reichl's scheme. Scheme (8.114a-b).

Similarly for the spin field, we set

$$S'(\boldsymbol{k}) = \begin{cases} \mathfrak{S}_L(\boldsymbol{k}) & \text{for} \quad \boldsymbol{k} \in R_{\mathfrak{S}} \\ \sigma_L(\boldsymbol{k}) & \text{for} \quad \boldsymbol{k} \in R_{\sigma} \end{cases} \tag{8.115-6}$$

The inverse transform [c.f. (8.107)] can therefore be written as

$$S'(\boldsymbol{x}) = \left(\frac{2\pi}{a}\right)^d \int_{\text{BZ}} d\,\boldsymbol{k}\, e^{i\,\boldsymbol{k}\cdot\boldsymbol{x}}\, S'(\boldsymbol{k}) \;= \mathfrak{S}_L(\boldsymbol{x}) + \sigma_L(\boldsymbol{x}) \tag{8.117a}$$

where

$$\mathfrak{S}_L(\boldsymbol{x}) = \left(\frac{2\pi}{a}\right)^d \int_{R_{\mathfrak{S}}} d\,\boldsymbol{k}\, e^{i\,\boldsymbol{k}\cdot\boldsymbol{x}}\, \mathfrak{S}_L(\boldsymbol{k}) \tag{8.117}$$

$$\sigma_L(\boldsymbol{x}) = \left(\frac{2\pi}{a}\right)^d \int_{R_\sigma} d\,\boldsymbol{k}\, e^{i\,\boldsymbol{k}\cdot\boldsymbol{x}}\, \sigma_L(\boldsymbol{k}) \tag{8.118}$$

Since $\mathfrak{S}_L(\boldsymbol{x})$ [$\sigma_L(\boldsymbol{x})$] is a superposition solely of plane waves with $\lambda > (<)\, L\, a$, it varies slowly (quickly) inside a block.

Caution: $\mathfrak{S}_L(\boldsymbol{x})$ [$\sigma_L(\boldsymbol{x})$] is not the inverse transform of $\mathfrak{S}_L(\boldsymbol{k})$ [$\sigma_L(\boldsymbol{k})$].

As in Ex.8.1, blocking is achieved by absorbing the internal (short wavelength) degrees of freedom into the coupling constants. Thus we write (8.113) as [c.f. (4) of Ex.8.1]

$$H = \mathcal{H}_{\mathfrak{S}} + \mathcal{H}_\sigma + V$$

where

$$\beta\mathcal{H}_{\mathfrak{S}}(r) = \frac{1}{2}\left(\frac{a}{2\pi}\right)^d \int_{R_{\mathfrak{S}}} d\,\boldsymbol{k}\,\left(k^2 + r\right)\left|\mathfrak{S}_L(\boldsymbol{k})\right|^2 \tag{8.119}$$

$$\beta\mathcal{H}_\sigma(r) = \frac{1}{2}\left(\frac{a}{2\pi}\right)^d \int_{R_\sigma} d\,\boldsymbol{k}\,\left(k^2 + r\right)\left|\sigma_L(\boldsymbol{k})\right|^2 \tag{8.120}$$

and

$$\beta\, V(u') = u'\left(\frac{a}{2\pi}\right)^{3d} \int_{\mathrm{BZ}} d\,\boldsymbol{k}_1 \int_{\mathrm{BZ}} d\,\boldsymbol{k}_2 \int_{\mathrm{BZ}} d\,\boldsymbol{k}_3 \int_{\mathrm{BZ}} d\,\boldsymbol{k}_4 \tag{8.121}$$
$$\times\, S'(\boldsymbol{k}_1)\, S'(\boldsymbol{k}_2)\, S'(\boldsymbol{k}_3)\, S'(\boldsymbol{k}_4)\, \delta(\boldsymbol{k}_1 + \boldsymbol{k}_2 + \boldsymbol{k}_3 + \boldsymbol{k}_4)$$

Next, we use $\mathcal{H}_\sigma$ to define the average

$$\langle A\{\mathfrak{S}_L\}\rangle = \frac{1}{Z_\sigma}\int \mathcal{D}\sigma_L\, e^{-\beta\mathcal{H}_\sigma}\, A(\{\mathfrak{S}_L,\, \sigma_L\}) \tag{8.122}$$

where

$$Z_\sigma = \int \mathcal{D}\sigma_L\, e^{-\beta\mathcal{H}_\sigma} \tag{8.122a}$$

is the partition function for the σ_L degrees of freedom.

(8.114) thus becomes

$$Z(r,\, u') = \int \mathcal{D}\,\mathfrak{S}_L \int \mathcal{D}\,\sigma_L\, e^{-\beta(\mathcal{H}_{\mathfrak{S}} + \mathcal{H}_\sigma + V)}$$
$$= Z_\sigma \int \mathcal{D}\,\mathfrak{S}_L\; e^{-\beta\mathcal{H}_{\mathfrak{S}}}\left\langle e^{-\beta V}\right\rangle$$
$$= Z_\sigma \int \mathcal{D}\,\mathfrak{S}_L\; \exp\left\{-\beta\left[\mathcal{H}_{\mathfrak{S}} + \langle V\rangle - \frac{1}{2}\beta\left(\left\langle V^2\right\rangle - \langle V\rangle^2\right) + \ldots\right]\right\} \tag{8.123}$$

where the last expression made use of the cumulant expansion [cf. (7) of Ex.8.1].

Treating (8.123) as the partition function for the $\mathfrak{S}_L$ degrees of freedom, we can write it as

$$Z(r,\, u') = \int \mathcal{D}\,\mathfrak{S}_L\; e^{-\beta\mathcal{H}_L(r,\, u',\, \{\mathfrak{S}_L\})}$$

where we have dropped the irrelevant "constant" Z_0 and

$$\mathcal{H}_L(r,\; u',\, \{\mathfrak{S}_L\}) = \mathcal{H}_{\mathfrak{S}} + \langle V\rangle - \frac{1}{2}\beta\left(\left\langle V^2\right\rangle - \langle V\rangle^2\right) + \ldots \tag{8.124}$$

The renormalized partition function is defined as

$$Z(r_L,\, u_L) \equiv \int \mathcal{D}\,\mathfrak{S}_L\, e^{-\beta H_L(r_L,\, u_L,\, \{\mathfrak{S}_L\})} \tag{8.124a}$$

where H_L is the renormalized Hamiltonian [cf. (8.113)]

$$\beta H_L\left(r_L,\, u_L,\, \{S_L\}\right) = \frac{1}{2}\left(\frac{a}{2\pi}\right)^d \int_{BZ} d\boldsymbol{k}\,\left(k^2 + r_L\right)\left|S_L(\boldsymbol{k})\right|^2 \tag{8.125}$$

$$+u_L\left(\frac{a}{2\pi}\right)^{3d} \int_{BZ} d\boldsymbol{k}_1 \int_{BZ} d\boldsymbol{k}_2 \int_{BZ} d\boldsymbol{k}_3 \int_{BZ} d\boldsymbol{k}_4$$

$$\times S_L(\boldsymbol{k}_1)\, S_L(\boldsymbol{k}_2)\, S_L(\boldsymbol{k}_3)\, S_L(\boldsymbol{k}_4)\, \delta\left(\boldsymbol{k}_1 + \boldsymbol{k}_2 + \boldsymbol{k}_3 + \boldsymbol{k}_4\right)$$

Setting

$$\mathcal{H}_L\left(r,\, u',\, \{\mathfrak{S}_L\}\right) = H\left(r_L,\, u_L,\, \{S_L\}\right) \tag{8.125a}$$

allows us to obtain $\{r_L, u_L\}$ in terms of $\{r, u'\}$ [cf. (13-4) of Ex.8.1].
In the absence of the S^4 term, i.e., $u' = 0$, (8.125a) gives

$$\int_{R_\mathfrak{S}} d\boldsymbol{k}\,\left(k^2 + r\right)\left|\mathfrak{S}_L(\boldsymbol{k})\right|^2 = \int_{BZ} d\boldsymbol{k}\,\left(k^2 + r_L\right)\left|S_L(\boldsymbol{k})\right|^2 \tag{8.125b}$$

Using

$$\int_{R_\mathfrak{S}} d\boldsymbol{k} = \int d\Omega \int_0^{\pi/a'L} dk\, k^{d-1}$$

$$= L^{-d} \int d\Omega \int_0^{\pi/a'} dk_L\, k_L^{d-1} \qquad k_L = L\,k \tag{8.132}$$

$$= L^{-d} \int_{BZ} d\boldsymbol{k} \tag{8.125c}$$

we can write (8.125b) as

$$L^{-d} \int_{BZ} d\boldsymbol{k}\,\left(k^2 L^{-2} + r\right)\left|\mathfrak{S}_L(\boldsymbol{k})\right|^2 = \int_{BZ} d\boldsymbol{k}\,\left(k^2 + r_L\right)\left|S_L(\boldsymbol{k})\right|^2 \tag{8.125d}$$

with solution

$$r_L = r\,L^2$$

$$S_L(\boldsymbol{k}) = L^{-(d/2+1)}\,\mathfrak{S}_L(\boldsymbol{k}) \tag{8.133}$$

The next step is to evaluate the cumulants of V for $u' \neq 0$.

To begin, breaking up each integral into a sum of long and short wavelength parts turns (8.121) into

$$\beta V(u') = u'\left(\frac{a}{2\pi}\right)^{3d} \prod_{j=1}^{4}\left(\int_{R_\mathfrak{S}} d\boldsymbol{k}_j\, \mathfrak{S}_L(\boldsymbol{k}_j) + \int_{R_\sigma} d\boldsymbol{k}_j\, \sigma_L(\boldsymbol{k}_j)\right) \delta(\boldsymbol{k}_1 + \boldsymbol{k}_2 + \boldsymbol{k}_3 + \boldsymbol{k}_4)$$

Since the $\boldsymbol{k}_j$'s are dummy variables, any permutation of them among the same type of fields will give the same numerical result. Therefore,

$$\beta\, V(u') = u' \left(\frac{a}{2\,\pi}\right)^{3\,d} \left\{ \prod_{j=1}^{4} \int_{R_{\mathfrak{S}}} d\,\boldsymbol{k}_j\, \mathfrak{S}_L(\boldsymbol{k}_j) + \prod_{j=1}^{4} \int_{R_\sigma} d\,\boldsymbol{k}_j\, \sigma_L(\boldsymbol{k}_j) \right. \tag{8.126a}$$

$$+ 4 \prod_{j=1}^{3} \int_{R_{\mathfrak{S}}} d\,\boldsymbol{k}_j\, \mathfrak{S}_L(\boldsymbol{k}_j) \int_{R_\sigma} d\,\boldsymbol{k}_4\, \sigma_L(\boldsymbol{k}_4)$$

$$+ 6 \prod_{j=1}^{2} \int_{R_{\mathfrak{S}}} d\,\boldsymbol{k}_j\, \mathfrak{S}_L(\boldsymbol{k}_j) \prod_{i=3}^{4} \int_{R_\sigma} d\,\boldsymbol{k}_i\, \sigma_L(\boldsymbol{k}_i)$$

$$\left. + 4 \prod_{j=1}^{3} \int_{R_\sigma} d\,\boldsymbol{k}_j\, \sigma_L(\boldsymbol{k}_j) \int_{R_{\mathfrak{S}}} d\,\boldsymbol{k}_4\, \mathfrak{S}_L(\boldsymbol{k}_4) \right\} \delta(\boldsymbol{k}_1 + \boldsymbol{k}_2 + \boldsymbol{k}_3 + \boldsymbol{k}_4)$$

where the coefficients are given by [cf. the binomial theorem]

$$4 = C_3^4 = \frac{4!}{3!\quad 1!} \qquad\qquad 6 = C_2^4 = \frac{4!}{2!\quad 2!}$$

The average (8.122) is a product of integrals

$$\langle A\,\{\mathfrak{S}_L\}\,\rangle = \frac{1}{Z_\sigma} \prod_{\boldsymbol{k}\in R_\sigma} \int_{\mathbb{C}} d\,\sigma_L\,(\boldsymbol{k})\, e^{-\beta\mathcal{H}_\sigma}\, A(\,\{\mathfrak{S}_L\,,\ \sigma_L(\boldsymbol{k})\}\,)$$

where $\mathbb{C}$ is the complex plane so that with

$$\sigma_L(\boldsymbol{k}) = \left|\ \sigma_L(\boldsymbol{k})\ \right|\ e^{i\,\phi} \equiv \rho_{\boldsymbol{k}}\, e^{i\,\phi} \tag{8.126b}$$

we have

$$\int_{\mathbb{C}} d\,\sigma_L(\boldsymbol{k}) = \int_0^{2\,\pi} d\,\phi \int_0^\infty d\,\rho_{\boldsymbol{k}}\, \rho_{\boldsymbol{k}}$$

Hence, for any function

$$f = f(\rho_{\boldsymbol{k}})$$

$$\int_{\mathbb{C}} d\,\sigma_L\,(\boldsymbol{k}) * \sigma_L\,(\boldsymbol{k})^m\ f\ = \int_0^{2\,\pi} d\,\phi\, e^{i\,m\,\phi} \int_0^\infty d\,\rho_{\boldsymbol{k}}\, {\rho_{\boldsymbol{k}}}^{m+1}\, f$$

$$= \delta_{m\,0}\, 2\,\pi \int_0^\infty d\,\rho_{\boldsymbol{k}}\, {\rho_{\boldsymbol{k}}}^{m+1}\, f \tag{8.126c}$$

Also,

$$\int_{\mathbb{C}} d\,\sigma_L\,(\boldsymbol{k}) * \sigma_L(\boldsymbol{k})\, \sigma_L(-\boldsymbol{k})\ f\ = \int_0^{2\,\pi} d\,\phi \int_0^\infty d\,\rho_{\boldsymbol{k}}\, \rho_{\boldsymbol{k}}^3\, f$$

$$= 2\,\pi \int_0^\infty d\,\rho_{\boldsymbol{k}}\, \rho_{\boldsymbol{k}}^3\, f$$

$$\rightarrow \qquad \int_{\mathbb{C}} d\,\sigma_L\,(\boldsymbol{k}) * \sigma_L(\boldsymbol{k})\, \sigma_L(\boldsymbol{k}')\ f\ = \delta_{\boldsymbol{k},-\boldsymbol{k}'}\, 2\,\pi \int_0^\infty d\,\rho_{\boldsymbol{k}}\, \rho_{\boldsymbol{k}}^3\, f$$

$$= \frac{(2\,\pi)^d}{V}\, \delta(\boldsymbol{k} + \boldsymbol{k}')\ 2\,\pi \int_0^\infty d\,\rho_{\boldsymbol{k}}\, \rho_{\boldsymbol{k}}^3\, f \tag{8.126d}$$

(8.120) can be written as

$$\beta\mathcal{H}_\sigma(r) = \beta \left(\frac{a}{2\,\pi}\right)^d \int_{R_\sigma} d\,\boldsymbol{k}\ \ h_\sigma(r,\, \boldsymbol{k}) \tag{8.126e}$$

where

$$\beta\ h_\sigma\,(r,\, \boldsymbol{k}) = \frac{1}{2} \left(k^2 + r\right) \left|\sigma_L(\boldsymbol{k})\right|^2$$

$$= \frac{1}{2}\left(k^2 + r\right)\rho_{\boldsymbol{k}}^2 \qquad (8.126f)$$

Hence,

$$Z_\sigma = \int \mathcal{D}\,\sigma_L\, e^{-\beta \mathcal{H}_\sigma}$$

$$= \left(\prod_{\boldsymbol{k}\in R_\sigma} \int_{\mathbb{C}} d\,\sigma_L(\boldsymbol{k})\right) \exp\left[-\beta\left(\frac{a}{2\pi}\right)^d \int_{R_\sigma} d\,\boldsymbol{k}\, h_\sigma(r, \boldsymbol{k})\right]$$

$$= \left(\prod_{\boldsymbol{k}\in R_\sigma} \int_{\mathbb{C}} d\,\sigma_L(\boldsymbol{k})\right) \exp\left[-\frac{\beta}{N} \sum_{\boldsymbol{k}\in R_\sigma} h_\sigma(r, \boldsymbol{k})\right]$$

$$= \prod_{\boldsymbol{k}\in R_\sigma} \left\{ \int_{\mathbb{C}} d\,\sigma_L\,(\boldsymbol{k}) \exp\left[-\frac{\beta}{N} h_\sigma(r, \boldsymbol{k})\right]\right\}$$

$$= \prod_{\boldsymbol{k}\in R_\sigma} z_\sigma(\boldsymbol{k}) \qquad (8.126g)$$

where

$$z_\sigma(\boldsymbol{k}) = \int_{\mathbb{C}} d\,\sigma_L\,(\boldsymbol{k}) \exp\left[-\frac{\beta}{N} h_\sigma(r, \boldsymbol{k})\right] \qquad (8.126g)$$

$$= 2\pi \int_0^\infty d\,\rho_{\boldsymbol{k}}\, \rho_{\boldsymbol{k}} \exp\left[-\frac{1}{2N}\left(k^2 + r\right)\rho_{\boldsymbol{k}}^2\right]$$

$$= \frac{2\pi N}{k^2 + r} \qquad \text{[See §Code.]} \qquad (8.126h)$$

We now return to the calculation of the average of (8.126a). To begin,

the term $\left\langle \prod_{j=1}^{4} \int_{R_\sigma} d\,\boldsymbol{k}_j\, \sigma_L(\boldsymbol{k}_j)\right\rangle$ can be dropped since it contributes only a constant (independent of $\mathfrak{S}_L$) to the renormalized Hamiltonian (8.124).

For the 3rd term in (8.126a), we have

$$\langle\, \sigma_L(\boldsymbol{k}_4)\,\rangle = \frac{1}{z_\sigma(\boldsymbol{k}_4)} \int_{\mathbb{C}} d\,\sigma_L(\boldsymbol{k}_4)\, \sigma_L(\boldsymbol{k}_4) \exp\left[-\frac{\beta}{N} h_\sigma\,(r, \boldsymbol{k}_4)\right]$$

$$= 0 \qquad \text{[See (8.126b) with } m = 1.\text{]} \qquad (8.127a)$$

For the 3rd term in (8.126a), we have

$$\int_{R_\sigma} d\,\boldsymbol{k}_3 \int_{R_\sigma} d\,\boldsymbol{k}_4\, \langle\, \sigma_L(\boldsymbol{k}_3)\, \sigma_L(\boldsymbol{k}_4)\,\rangle$$

$$= \int_{R_\sigma} d\,\boldsymbol{k}_3 \int_{R_\sigma} d\,\boldsymbol{k}_4\, \delta_{\boldsymbol{k}_3, -\boldsymbol{k}_4} \langle\, \sigma_L(\boldsymbol{k}_3)\, \sigma_L(-\boldsymbol{k}_3)\,\rangle \qquad \text{[(8.126d) used.]}$$

$$= \int_{R_\sigma} d\,\boldsymbol{k}_3 \int_{R_\sigma} d\,\boldsymbol{k}_4\, \frac{(2\pi)^d}{V} \delta(\boldsymbol{k}_3 + \boldsymbol{k}_4) \langle\, \sigma_L(\boldsymbol{k}_3)\, \sigma_L(-\boldsymbol{k}_3)\,\rangle$$

$$= \frac{(2\pi)^d}{V} \int_{R_\sigma} d\,\boldsymbol{k}_3\, \langle\, \sigma_L(\boldsymbol{k}_3)\, \sigma_L(-\boldsymbol{k}_3)\,\rangle$$

$$= \frac{(2\pi)^d}{V} \int_{R_\sigma} d\,\boldsymbol{k}_3\, \frac{1}{z_\sigma(\boldsymbol{k}_3)} 2\pi \int_0^\infty d\,\rho_{\boldsymbol{k}_3}\, \rho_{\boldsymbol{k}_3}^3 \exp\left[-\frac{1}{2N}\left(k_3^2 + r\right)\rho_{\boldsymbol{k}_3}^2\right]$$

$$= \frac{(2\pi)^d}{V} \int_{R_\sigma} d\,\boldsymbol{k}_3 \; \frac{1}{z_\sigma(\boldsymbol{k}_3)} \, 2\pi \, \frac{2N^2}{\left(k_3^2 + r\right)^2} \qquad \text{[See §Code.]}$$

$$= \left(\frac{2\pi}{a}\right)^d \int_{R_\sigma} d\,\boldsymbol{k}_3 \; \frac{2}{k_3^2 + r} \qquad (8.127\text{b})$$

This can also be represented as

$$\langle \sigma_L(\boldsymbol{k}_3)\, \sigma_L(\boldsymbol{k}_4) \rangle = \frac{(2\pi)^d}{V} \delta(\boldsymbol{k}_3 + \boldsymbol{k}_4) \langle \sigma_L(\boldsymbol{k}_3)\, \sigma_L(-\boldsymbol{k}_3) \rangle$$

$$= \delta(\boldsymbol{k}_3 + \boldsymbol{k}_4) \left(\frac{2\pi}{a}\right)^d \frac{2}{k_3^2 + r} \qquad (8.127)$$

For the 4th term in (8.126a), we have

$$\int_{R_\sigma} d\,\boldsymbol{k}_1 \int_{R_\sigma} d\,\boldsymbol{k}_2 \int_{R_\sigma} d\,\boldsymbol{k}_3 \langle \sigma_L(\boldsymbol{k}_1)\, \sigma_L(\boldsymbol{k}_2)\, \sigma_L(\boldsymbol{k}_3) \rangle = 0 \qquad (8.127\text{c})$$

since there is no way to write the integrand as a pure function of $\rho_{\boldsymbol{k}}$.

Note: it is straight forward to generalize the above results and derive the Wick's theorem [see Ex.4.9, part (c)],

$$\langle \sigma_L(\boldsymbol{k}_1) \ldots \sigma_L(\boldsymbol{k}_{2n}) \rangle$$
$$= \langle \sigma_L(\boldsymbol{k}_1)\, \sigma_L(\boldsymbol{k}_2) \rangle \ldots \langle \sigma_L(\boldsymbol{k}_{2n-1})\, \sigma_L(\boldsymbol{k}_{2n}) \rangle + \text{ permutations}$$
$$= \delta_{\boldsymbol{k}_1, -\boldsymbol{k}_2} \ldots \delta_{\boldsymbol{k}_{2n-1}, -\boldsymbol{k}_{2n}} \langle \sigma_L(\boldsymbol{k}_1)\, \sigma_L(-\boldsymbol{k}_1) \rangle \ldots \langle \sigma_L(\boldsymbol{k}_{2n-1})\, \sigma_L(-\boldsymbol{k}_{2n-1}) \rangle \qquad (8.127\text{d})$$
$$+ \text{ permutations}$$

The average of (8.126a) then gives

$$\beta \langle V(u') \rangle = u' \left(\frac{a}{2\pi}\right)^{3d} \left\{ \prod_{j=1}^{4} \int_{R_{\mathfrak{S}}} d\,\boldsymbol{k}_j \, \mathfrak{S}_L(\boldsymbol{k}_j)\, \delta(\boldsymbol{k}_1 + \boldsymbol{k}_2 + \boldsymbol{k}_3 + \boldsymbol{k}_4) \right. \qquad (8.128)$$

$$\left. + 6 \prod_{j=1}^{2} \int_{R_{\mathfrak{S}}} d\,\boldsymbol{k}_j \, \mathfrak{S}_L(\boldsymbol{k}_j) \left(\frac{2\pi}{a}\right)^d \int_{R_\sigma} d\,\boldsymbol{k}_3 \, \frac{2}{k_3^2 + r} \delta(\boldsymbol{k}_1 + \boldsymbol{k}_2) \right\}$$

$$= u' \left(\frac{a}{2\pi}\right)^{3d} \int_{R_{\mathfrak{S}}} d\,\boldsymbol{k}_1 \int_{R_{\mathfrak{S}}} d\,\boldsymbol{k}_2 \int_{R_{\mathfrak{S}}} d\,\boldsymbol{k}_3 \int_{R_{\mathfrak{S}}} d\,\boldsymbol{k}_4 \qquad (8.128\text{a})$$
$$\times \mathfrak{S}_L(\boldsymbol{k}_1)\, \mathfrak{S}_L(\boldsymbol{k}_2)\, \mathfrak{S}_L(\boldsymbol{k}_3)\, \mathfrak{S}_L(\boldsymbol{k}_4)\, \delta(\boldsymbol{k}_1 + \boldsymbol{k}_2 + \boldsymbol{k}_3 + \boldsymbol{k}_4)$$
$$+ 6\, u' \left(\frac{a}{2\pi}\right)^{2d} \int_{R_\sigma} d\,\boldsymbol{k}_3 \, \frac{2}{k_3^2 + r} \int_{R_{\mathfrak{S}}} d\,\boldsymbol{k}_1 \, \mathfrak{S}_L(\boldsymbol{k}_1)\, \mathfrak{S}_L(-\boldsymbol{k}_1)$$

Under the scale change $k = k_L / L$, we have

$$\delta(\boldsymbol{k}) = \prod_{i=1}^{d} \delta(k_i) = \prod_{i=1}^{d} \delta\left(\frac{k_{L\,i}}{L}\right) = \prod_{i=1}^{d} L\, \delta(k_{L\,i}) = L^d\, \delta(\boldsymbol{k}_L) \qquad (8.128\text{b})$$

Using (8.125c), (8.133) & (8.128b), we have

$$\beta \langle V(u') \rangle = u' \left(\frac{a}{2\pi}\right)^{3d} L^{-4d} \int_{\mathrm{BZ}} d\,\boldsymbol{k}_1 \int_{\mathrm{BZ}} d\,\boldsymbol{k}_2 \int_{\mathrm{BZ}} d\,\boldsymbol{k}_3 \int_{\mathrm{BZ}} d\,\boldsymbol{k}_4$$
$$\times L^{2d+4}\, S_L(\boldsymbol{k}_1)\, S_L(\boldsymbol{k}_2)\, S_L(\boldsymbol{k}_3)\, S_L(\boldsymbol{k}_4)\, L^d\, \delta(\boldsymbol{k}_1 + \boldsymbol{k}_2 + \boldsymbol{k}_3 + \boldsymbol{k}_4)$$
$$+ 6\, u' \left(\frac{a}{2\pi}\right)^{2d} \int_{R_\sigma} d\,\boldsymbol{k}_3 \, \frac{2}{k_3^2 + r} L^{-d} \int_{\mathrm{BZ}} d\,\boldsymbol{k}_1 \, L^{d+2}\, S_L(\boldsymbol{k}_1)\, S_L(-\boldsymbol{k}_1)$$

$$= u' \, L^{4-d} \left(\frac{a}{2\pi}\right)^{3d} \int_{\mathrm{BZ}} d\boldsymbol{k}_1 \int_{\mathrm{BZ}} d\boldsymbol{k}_2 \int_{\mathrm{BZ}} d\boldsymbol{k}_3 \int_{\mathrm{BZ}} d\boldsymbol{k}_4 \tag{8.128c}$$

$$\times S_L(\boldsymbol{k}_1)\, S_L(\boldsymbol{k}_2)\, S_L(\boldsymbol{k}_3)\, S_L(\boldsymbol{k}_4)\, \delta(\boldsymbol{k}_1 + \boldsymbol{k}_2 + \boldsymbol{k}_3 + \boldsymbol{k}_4)$$

$$+ \frac{1}{2} u' \, L^2 \int_{R_\sigma} d\boldsymbol{k}_3 \frac{24}{k_3^2 + r} \left(\frac{a}{2\pi}\right)^{2d} \int_{\mathrm{BZ}} d\boldsymbol{k}_1\, S_L(\boldsymbol{k}_1)\, S_L(-\boldsymbol{k}_1)$$

The 1st term in (8.128c) gives

$$u_L = L^{4-d} u' \tag{8.136a}$$

while the 2nd term modifies (8.125e) to

$$r_L = L^2 \left[r + 24\, u' \left(\frac{a}{2\pi}\right)^d \int_{R_\sigma} d\boldsymbol{k} \frac{1}{k^2 + r} \right] \tag{8.135a}$$

The following differs from Reichl's text sufficiently to warrant a different set of equation labels.

In order to find the fixed point, we need to identify the transformation that satisfies the group multiplication property (8.84). Since L is continuous, we are dealing with a Lie (or continuous) semi-group. Hence, the transformation is of the form

$$T(L) = e^{(L-1)\boldsymbol{J}} \qquad [\text{ Identity transformation is } T(1) = \boldsymbol{I}. \,] \tag{B.1}$$

where $\boldsymbol{J}$ is the generator that acts on the space $(r,\, u)$ so that (8.136a) & (8.135a) become

$$\begin{pmatrix} r_L \\ u_L \end{pmatrix} = e^{(L-1)\boldsymbol{J}} \begin{pmatrix} r \\ u' \end{pmatrix} \tag{B.2}$$

As usual, $\boldsymbol{J}$ is obtained by considering the infinitesimal transformation

$$T(1+h) = e^{h\boldsymbol{J}} \approx \boldsymbol{I} + h\,\boldsymbol{J} \qquad h \to 0$$

so that

$$\begin{pmatrix} r_{1+h} \\ u_{1+h} \end{pmatrix} \approx (\boldsymbol{I} + h\,\boldsymbol{J}) \begin{pmatrix} r \\ u' \end{pmatrix}$$

$$= \begin{pmatrix} r \\ u' \end{pmatrix} + h \begin{pmatrix} J_{rr} & J_{ru} \\ J_{ur} & J_{uu} \end{pmatrix} \begin{pmatrix} r \\ u' \end{pmatrix} \qquad \boldsymbol{J} = \begin{pmatrix} J_{rr} & J_{ru} \\ J_{ur} & J_{uu} \end{pmatrix}$$

$$= \begin{pmatrix} r + h\,(J_{rr}\, r + J_{ru}\, u') \\ u' + h\,(J_{ur}\, r + J_{uu}\, u') \end{pmatrix} \tag{B.3}$$

Meanwhile, (8.136a) & (8.135a) gives

$$u_{1+h} = (1+h)^{4-d} u'$$

$$\approx u' + (4-d)\, h\, u' \tag{B.4}$$

$$r_{1+h} = (1+h)^2 \left[r + 24\, u' \left(\frac{a}{2\pi}\right)^d \Omega_{d-1} \int_{\pi/a'(1+h)}^{\pi/a'} dk \frac{k^{d-1}}{k^2 + r} \right] \tag{B.5}$$

where Ω_d [see (A.21)] is the surface area of a d-sphere of unit radius.

Using

$$\int_{\pi/a'(1+h)}^{\pi/a'} dk \frac{k^{d-1}}{k^2 + r} \approx h \frac{(\pi/a')^d}{(\pi/a')^2 + r}$$

(B.5) becomes

$$r_{1+h} \approx (1 + 2h) \left[r + 24\, u' \left(\frac{a}{2\pi}\right)^d \Omega_{d-1}\, h \frac{(\pi/a')^d}{(\pi/a')^2 + r} \right]$$

$$\approx r + h\left[2r + 24u'\left(\frac{a}{2\pi}\right)^d \Omega_{d-1} \frac{(\pi/a')^d}{(\pi/a')^2 + r}\right] \tag{B.6}$$

Using (A.22), we can write (8.114a) as

$$\frac{1}{d}\left(\frac{\pi}{a'}\right)^d \Omega_{d-1} = \left(\frac{2\pi}{a}\right)^d$$

so that (B.6) becomes

$$r_{1+h} \approx r + h\left(2r + 24u' \frac{d}{(\pi/a')^2 + r}\right) \tag{B.7}$$

Comparing (B.4) & (B.7) with (b.3) gives

$$\boldsymbol{J} = \begin{pmatrix} 2 & \frac{24d}{(\pi/a')^2 + r} \\ 0 & 4 - d \end{pmatrix} \tag{B.8}$$

The fixed points of the transformation are given by

$$\begin{pmatrix} r^* \\ u^* \end{pmatrix} = T(L)\begin{pmatrix} r^* \\ u^* \end{pmatrix} \tag{B.9}$$

Consider a nearby point

$$\begin{pmatrix} r \\ u \end{pmatrix} = \begin{pmatrix} r^* \\ u^* \end{pmatrix} + \begin{pmatrix} \delta r \\ \delta u \end{pmatrix}$$

Operating with $T(1+h)$ gives

$$\begin{pmatrix} r_{1+h} \\ u_{1+h} \end{pmatrix} = \begin{pmatrix} r^* \\ u^* \end{pmatrix} + (\boldsymbol{I} + h\boldsymbol{J})\begin{pmatrix} \delta r \\ \delta u \end{pmatrix} = \begin{pmatrix} r \\ u \end{pmatrix} + h\boldsymbol{J}\begin{pmatrix} \delta r \\ \delta u \end{pmatrix}$$

Hence

$$\frac{1}{h}\left[\begin{pmatrix} r_{1+h} \\ u_{1+h} \end{pmatrix} - \begin{pmatrix} r \\ u \end{pmatrix}\right] = \boldsymbol{J}\begin{pmatrix} \delta r \\ \delta u \end{pmatrix}$$

$$\rightarrow \qquad \frac{\partial}{\partial L}\begin{pmatrix} r_L \\ u_L \end{pmatrix}\bigg|_{L=1} = \boldsymbol{J}\begin{pmatrix} \delta r \\ \delta u \end{pmatrix} \qquad \text{for } h \to 0 \tag{B.10}$$

Since $\delta r = \delta u = 0$ at the fixed point,

$$\frac{\partial}{\partial L}\begin{pmatrix} r_L^* \\ u_L^* \end{pmatrix}\bigg|_{L=1} = 0 \tag{B.11}$$

Putting (8.135a) and (8.136a) into (B.9) gives

$$u_L^* = L^{4-d} u^* \tag{B.12}$$

$$r_L^* = L^2\left[r^* + 24u^*\left(\frac{a}{2\pi}\right)^d \int_{R_\sigma} d\boldsymbol{k} \frac{1}{k^2 + r^*}\right]$$

$$= L^2\left[r^* + 24u^*\left(\frac{a}{2\pi}\right)^d \Omega_{d-1} \int_{\pi/a'L}^{\pi/a'} dk \frac{k^{d-1}}{k^2 + r}\right] \tag{B.13}$$

Applying (B.11) to (B.12) gives

$$(4-d)u^* = 0$$

$$\rightarrow \qquad u^* = \begin{cases} 0 & \text{if } d \neq 4 \\ \text{arbitrary} & \text{if } d = 4 \end{cases} \tag{B.14}$$

Taking advantage of the fixed point property $r_L^* = r^*$, (B.13) gives

$$2\, r^* + 24\, u^* \left(\frac{a}{2\,\pi}\right)^d \Omega_{d-1} \left(\frac{\partial}{\partial L} \int_{\pi/a' L}^{\pi/a'} d\,k\, \frac{k^{d-1}}{k^2 + r}\right)_{L=1} = 0$$

Using

$$\frac{\partial}{\partial L}\left(\int_{\text{const}}^{g(L)} f(x)\, d\,x\right) = \frac{d\,g(L)}{d\,L}\, f[\,g(L)\,]$$

we have

$$2\, r^* + 24\, u^* \left(\frac{a}{2\,\pi}\right)^d \Omega_{d-1}\, \frac{\pi}{a'}\, \frac{(\pi/a')^{d-1}}{(\pi/a')^2 + r} = 0$$

$$\rightarrow \qquad 2\, r^* + 24\, u^* \frac{d}{(\,\pi/a'\,)^2 + r^*} = 0 \qquad \text{[See (B.7)]} \qquad \text{(B.15)}$$

Combing (B.14) with (B.15) gives

$$(r^*,\, u^*) = (0,\, 0) \qquad \text{if} \quad d \neq 4 \qquad \text{(B.16)}$$

For $d = 4$, the “fixed point” becomes a curve given by (B.15). We shall not attempt to interpret this since inclusion of higher order cumulants of V will remove it.

Putting (B.8) into (B.10) gives

$$\begin{pmatrix} \frac{\partial r_L}{\partial L} \\ \frac{\partial u_L}{\partial L} \end{pmatrix}_{L=1} = \begin{pmatrix} 2 & \frac{24\, d}{(\,\pi/a'\,)^2 + r} \\ 0 & 4 - d \end{pmatrix} \begin{pmatrix} \delta\, r \\ \delta\, u \end{pmatrix} \qquad \text{(B.17)}$$

which can be used to analyze the characteristics of the fixed points. (B.17) is the 1st cumulant approximation to (8.149) in Reichl’s text.

Note that the fixed point equations (B.14-5) can be expressed as

$$\boldsymbol{J} \begin{pmatrix} r^* \\ u^* \end{pmatrix} = 0 \qquad \text{(B.18)}$$

which can be obtained directly from (B.9) with $T(L) = T(1 + h) = \boldsymbol{I} + h\, \boldsymbol{J}$.

In terms of the language used in §8.D, the generator $\boldsymbol{J}$ is equivalent to the linearized transformation matrix $\mathbb{A}$ of (8.87).

The eigenvalues of $\boldsymbol{J}$ thus give the critical exponents according to (8.96-7). However, both r and u' are temperature parameters (via β) so that $\boldsymbol{J}$ can only provide the exponent p.

The eigensystem of $\boldsymbol{J}$ at the fixed point $(r^*,\, u^*) = (0,\, 0)$ gives [see §Code]

$$\lambda_1 = 2 \qquad v_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad \text{(B.19)}$$

$$\lambda_2 = 4 - d \qquad v_2 = \begin{pmatrix} \frac{24\, d}{(\,\pi/a'\,)^2} \\ 2 - d \end{pmatrix} \qquad \text{(B.20)}$$

From $T(1 + h) = e^{h\, \boldsymbol{J}}$, we see that the fixed point is repulsive (attractive) along the eigenvector of an eigenvalue that is positive (negative). Hence, for $d < 4$, both eigenvalues are positive and the fixed point is unreachable and hence unphysical. For $d > 4$, the fixed point is physical while the repulsive eigenvalue λ_1 is relevant.

Consider a point $\epsilon_j\, v_j$ on the eigenvector v_j. Under the transformation $T(L)$, we have

$$\epsilon_{j\,L}\, v_j = T(L)\, \epsilon_j\, v_j \; = e^{(L-1)\, \boldsymbol{J}}\, \epsilon_j\, v_j \; = e^{\lambda_j (L-1)}\, \epsilon_j\, v_j$$

$$\rightarrow \qquad \epsilon_{j\,L} = e^{\lambda_j (L-1)}\, \epsilon_j$$

The singular part of the free energy density thus scales like [cf. (8.93)]

$$g_s(\epsilon_1, \epsilon_2, \ldots) = L^{-d} g_s(\epsilon_{1L}, \epsilon_{2L}, \ldots)$$
$$= L^{-d} g_s\left(e^{\lambda_1 (L-1)} \epsilon_1, e^{\lambda_2 (L-1)} \epsilon_2, \ldots\right)$$

Comparing with the Widom scaling

$$g_s(\epsilon, B, \ldots) = \frac{1}{\alpha} g_s(\alpha^p \epsilon, \alpha^q B, ..)$$

we have, for $d > 4$,

ϵ_2 is dropped as irrelevant,

$\epsilon = \epsilon_1 \qquad \alpha = L^d \qquad \alpha^p = e^{\lambda_1 (L-1)}$

$\to \qquad p \ln \alpha = \lambda_1 (L-1)$
$= p\, d \ln L$

Since the basic transformation is $L = 1 + h$ with $h \to 0$, we have

$$p = \lim_{L \to 1} \frac{\lambda_1 (L-1)}{d \ln L} = \lim_{L \to 1} \frac{\lambda_1}{d\, L^{-1}} = \frac{\lambda_1}{d} = \frac{2}{d} \qquad d > 4 \qquad \text{(B.21)}$$

which is the 1st cumulant approximation to (8.153) in Reichl's text. In fact, (B.21) is the same as (8.153) since $u^* = 0$ for the fixed point $(r^*, u^*) = (0, 0)$.

Other critical exponents that depend only on p are

$$\alpha = 2 - \frac{1}{p} = 2 - \frac{d}{2} \qquad \text{[see (8.50)]} \qquad \text{(B.22)}$$

$$\nu = \frac{2 - \alpha}{d} = \frac{1}{2} \qquad \text{[see (8.77)]} \qquad \text{(B.23)}$$

which are 1st cumulant approximations to (8.156) and (8.159) in Reichl's text. However, like (B.21), the approximation is exact.

The inclusion of the 2nd cumulant $\langle V^2 \rangle - \langle V \rangle^2$ is necessary to obtain the 2nd fixed point, which is physical for $d < 4$ [see Fig.8.4 in Reichl's text]. However, the calculation, although straight forward, is rather lengthy. Since it requires no additional mathematical technique nor new physical concept, we shall leave it as an exercise.

Appendix

For a d-D cubic lattice with primitive lattice vectors

$$\boldsymbol{a}_i = a\, \hat{\boldsymbol{x}}_i \, i = 1, \ldots, d \qquad \text{(A.1)}$$

the site label $\boldsymbol{n}$ is a d-tuple of integers

$$\boldsymbol{n} = (n_1, \ldots, n_d) \qquad n_i = -M, \ldots, M-1 \qquad \text{(A.2)}$$

where M is an integer satisfying

$$(2M)^d = N = \text{number of sites}$$

The spatial position of site $\boldsymbol{n}$ is therefore

$$\boldsymbol{x} = \sum_{i=1}^{d} n_i \boldsymbol{a}_i = \sum_{i=1}^{d} n_i\, a\, \hat{\boldsymbol{x}}_i = \boldsymbol{n}\, a \qquad \text{(A.3)}$$

Assuming periodic boundary conditions [see (A.6)], we can expand $S_{\boldsymbol{n}}$ as a Fourier series

$$S_{\boldsymbol{n}} = \frac{1}{N} \sum_{\boldsymbol{k}} S_{\boldsymbol{k}}\, e^{i\,\boldsymbol{k}\cdot\boldsymbol{n}\,a} \qquad (A.4)$$

Comment:

1. $S_{\boldsymbol{n}}$ & $S_{\boldsymbol{k}}$ have the same dimensions (both are dimensionless).

2. Since $S_{\boldsymbol{k}}$ is merely a mathematical construct to help describe the physical quantity $S_{\boldsymbol{n}}$, the choice of the prefactor, $1/N$, is purely a matter of convenience. For the same reason, $S_{\boldsymbol{n}}$ must be real but $S_{\boldsymbol{k}}$ can be complex, with $S_{\boldsymbol{k}}^* = S_{-\boldsymbol{k}}$.

Let $\boldsymbol{e}_i$ be the d-tuple of integers whose only non-zero component, of value 1, is at the i^{th} position, i.e.,

$$\boldsymbol{e}_1 = (1, 0, 0, \ldots) \qquad \boldsymbol{e}_2 = (0, 1, 0, \ldots) \qquad \text{etc} \qquad (A.5)$$

then

$$\boldsymbol{n} = \sum_{i=1}^{d} n_i\, \boldsymbol{e}_i$$

The periodic boundary conditions [note that M is outside the lattice (A.2)]

$$S_{-M\,\boldsymbol{e}_i} = S_{M\,\boldsymbol{e}_i} \qquad i = 1, \ldots, d \qquad (A.6)$$

require

$$e^{-i\,k_i\,M\,a} = e^{i\,k_i\,M\,a} \qquad \rightarrow \qquad e^{2\,i\,k_i\,M\,a} = 1$$

$$\rightarrow \qquad 2\,k_i\,M\,a = 2\,\pi\,m_i \qquad m_i = \text{integers}$$

so that

$$k_i = \frac{m_i\,\pi}{M\,a} \qquad m_i = -M, \ldots, M-1 \qquad (A.7)$$

gives us $2\,M$ k_i points as counterparts to the $2\,M$ site points n_i. The region

$$-\frac{\pi}{a} \le k_i < \frac{\pi}{a} \qquad i = 1, \ldots, d \qquad (A.8)$$

is called the Brillouin zone (BZ). k_i outside BZ is equivalent to one inside given by

$$k_i + \frac{2\,\pi}{a}\,n \qquad \text{for some integer } n. \qquad (A.9)$$

(A.4) thus becomes

$$S_{\boldsymbol{n}} = \frac{1}{N} \sum_{\boldsymbol{k}\in \text{BZ}} S_{\boldsymbol{k}}\, e^{i\,\boldsymbol{k}\cdot\boldsymbol{n}\,a} \qquad (A.10)$$

Comments:

1. From the mathematical point of view, (A.10) remains valid if the BZ is replaced by any region of the same volume, i.e.,

$$-\frac{\pi}{a} + K_i \le k_i < \frac{\pi}{a} + K_i \qquad K_i \text{ arbitrary}$$

2. If we interpret (A.10) as a linear combination of plane waves with wavelengths $\lambda = \dfrac{2\,\pi}{|\,\boldsymbol{k}\,|}$, the BZ is equivalent to

$$0 \le k_i < \frac{2\,\pi}{a}$$

Waves with the shortest wavelength thus propagate along the x_i-axes with $\lambda = a$. Waves with $\lambda < a$ are indistinguishable from some waves with $\lambda > a$ [see (A.9)] when measurements are taken only at the lattice sites. A less accurate (but often used) way to describe this is to say that waves with $\lambda < a$ cannot propagate inside the lattice.

Now,

$$\sum_{n=-M}^{M-1} e^{\pm i k n a} = \sum_{n=-M}^{M-1} e^{\pm i m n \pi / M} \qquad k = \frac{m \pi}{M a} \qquad \text{[See (A.7).]}$$

$$= \frac{e^{\mp i m \pi} - e^{\pm i m \pi}}{1 - e^{\pm i m \pi / M}}$$

$$= \begin{cases} \dfrac{(-)^m - (-)^m}{1 - e^{\pm i m \pi / M}} & \text{for } m \neq 0 \\ \dfrac{1 \mp i m \pi + \ldots - (1 \pm i m \pi + \ldots)}{1 - (1 \pm i m \pi / M + \ldots)} & \text{for } m = 0 \end{cases}$$

$$= \begin{cases} 0 & \text{for } m \neq 0 \\ 2 M = N^{1/d} & \text{for } m = 0 \end{cases}$$

$$= N^{1/d} \delta_{k0}$$

$$\rightarrow \qquad \sum_{\boldsymbol{n}} e^{\pm i \boldsymbol{k} \cdot \boldsymbol{n} a} = \sum_{n_1} \ldots \sum_{n_d} e^{\pm i k_1 n_1 a} \ldots e^{\pm i k_d n_d a}$$

$$= N \delta_{k_1 0} \ldots \delta_{k_d 0} = N \delta_{\boldsymbol{k} 0} \tag{A.11}$$

$\sum_{\boldsymbol{n}} S_{\boldsymbol{n}} e^{-i \boldsymbol{k'} \cdot \boldsymbol{n} a} \times$(A.10) gives

$$\sum_{\boldsymbol{n}} S_{\boldsymbol{n}} e^{-i \boldsymbol{k'} \cdot \boldsymbol{n} a} = \frac{1}{N} \sum_{\boldsymbol{k} \in \mathrm{BZ}} S_{\boldsymbol{k}} \sum_{\boldsymbol{n}} e^{i (\boldsymbol{k} - \boldsymbol{k'}) \cdot \boldsymbol{n} a} = \sum_{\boldsymbol{k} \in \mathrm{BZ}} S_{\boldsymbol{k}} \delta_{\boldsymbol{k} \boldsymbol{k'}} = S_{\boldsymbol{k'}}$$

The inverse of (A.10) is therefore,

$$S_{\boldsymbol{k}} = \sum_{\boldsymbol{n}} S_{\boldsymbol{n}} e^{-i \boldsymbol{k} \cdot \boldsymbol{n} a} \tag{A.12}$$

The following identities are essential to manipulating Fourier series.

$$\int_{-\pi/a}^{\pi/a} d k \, e^{i k n a} = \frac{1}{i n a} \left(e^{i \pi n} - e^{-i \pi n} \right)$$

$$= \begin{cases} \frac{1}{i n a} [(-)^n - (-)^n] & \text{for } n \neq 0 \\ \frac{1}{i n a} [1 + i \pi n + \ldots - (1 - i \pi n + \ldots)] & \text{for } n = 0 \end{cases}$$

$$= \begin{cases} 0 & \text{for } n \neq 0 \\ \frac{2 \pi}{a} & \text{for } n = 0 \end{cases}$$

$$= \frac{2 \pi}{a} \delta_{n 0}$$

$$\rightarrow \qquad \int_{\mathrm{BZ}} d \boldsymbol{k} \, e^{i \boldsymbol{k} \cdot \boldsymbol{n} a} = \left(\frac{2 \pi}{a} \right)^d \prod_{i=1}^{d} \delta_{n_i 0} = \left(\frac{2 \pi}{a} \right)^d \delta_{\boldsymbol{n} 0} \tag{A.13}$$

where the integration over the Brillouin zone is defined as

$$\int_{\mathrm{BZ}} d \boldsymbol{k} = \prod_{i=1}^{d} \int_{-\pi/a}^{\pi/a} d k_i \tag{A.14}$$

Now,

$$\Delta k = \frac{\pi}{M a} \Delta m = \frac{2 \pi}{N^{1/d} a} \Delta m$$

$$\to \qquad \Delta \boldsymbol{k} = \Delta k_1 \ldots \Delta k_d = \frac{(2\pi)^d}{N a^d} \Delta m_1 \ldots \Delta m_d$$
$$= \frac{(2\pi)^d}{V} \Delta \boldsymbol{m} \qquad\qquad (\ V = N a^d = \text{volume of system}\ )$$

The volume occupied by 1 state is equal to $\Delta \boldsymbol{k} \mid_{\Delta \boldsymbol{m}=1}$. The density of state in k-space is therefore

$$\rho(\boldsymbol{k}) = \frac{V}{(2\pi)^d} \qquad \to \qquad \sum_{\boldsymbol{k}} = \int d\,\boldsymbol{k}\,\rho(\boldsymbol{k}) = \frac{V}{(2\pi)^d} \int d\,\boldsymbol{k} \qquad \text{(A.15)}$$

Assuming $f(\boldsymbol{k}) = f_{\boldsymbol{k}}$ at all discrete $\boldsymbol{k}$ points allowed for $f_{\boldsymbol{k}}$, then

$$\sum_{\boldsymbol{k}} f_{\boldsymbol{k}}\, \delta_{\boldsymbol{k}\boldsymbol{k}'} = f_{\boldsymbol{k}'} = f(\boldsymbol{k}') = \int d\,\boldsymbol{k}\, f(\boldsymbol{k})\, \delta(\boldsymbol{k} - \boldsymbol{k}')$$
$$= \frac{V}{(2\pi)^d} \int d\,\boldsymbol{k}\, f_{\boldsymbol{k}}\, \delta_{\boldsymbol{k}\boldsymbol{k}'} = \frac{V}{(2\pi)^d} \int d\,\boldsymbol{k}\, f(\boldsymbol{k})\, \delta_{\boldsymbol{k}\boldsymbol{k}'}$$

Therefore,

$$\delta(\boldsymbol{k} - \boldsymbol{k}') = \frac{V}{(2\pi)^d}\, \delta_{\boldsymbol{k}\boldsymbol{k}'} = N\left(\frac{a}{2\pi}\right)^d \delta_{\boldsymbol{k}\boldsymbol{k}'} \qquad \text{(A.16)}$$

(A.11) thus becomes

$$\sum_{\boldsymbol{n}} e^{\pm i\,\boldsymbol{k}\cdot\boldsymbol{n}\,a} = N\, \frac{(2\pi)^d}{V}\, \delta(\boldsymbol{k})$$
$$= \left(\frac{2\pi}{a}\right)^d \delta(\boldsymbol{k}) \qquad \text{(A.17)}$$

To check for consistency, we apply the procedure above to $\boldsymbol{x}$, starting with

$$\Delta \boldsymbol{x} = \Delta \boldsymbol{n}\ a$$
$$\to \qquad \rho(\boldsymbol{x}) = \frac{1}{\mid \Delta \boldsymbol{x} \mid_{\Delta \boldsymbol{n}=1}} = \frac{1}{a^d}$$
$$\therefore \qquad \sum_{\boldsymbol{n}} = \int_V d\,\boldsymbol{x}\, \rho(\boldsymbol{x}) = \frac{1}{a^d} \int_V d\,\boldsymbol{x} \qquad \text{(A.18)}$$

Treating $\boldsymbol{k}$ as discrete, we have

$$\sum_{\boldsymbol{n}} e^{-i\,\boldsymbol{k}\cdot\boldsymbol{n}\,a} = \frac{1}{a^d} \int_V d\,\boldsymbol{x}\, e^{-i\,\boldsymbol{k}\cdot\boldsymbol{x}} = \frac{V}{a^d}\, \delta_{\boldsymbol{k}0} = N\, \delta_{\boldsymbol{k}0}$$

in agreement with (A.11).

$$\int_V d\,\boldsymbol{x}\, e^{-i\,\boldsymbol{k}\cdot\boldsymbol{x}} = \prod_{j=1}^{d} \int_{-M a}^{M a} d\,x_j\, e^{-i\,k_j\,x_j} \qquad [\ V = (2 M a)^d\ ]$$
$$= \prod_{j=1}^{d} \frac{e^{-i\,k_j\,M a} - e^{i\,k_j\,M a}}{-i\,k_j}$$
$$= \prod_{j=1}^{d} \frac{e^{-i\,m_j\,\pi} - e^{i\,m_j\,\pi}}{-i\,m_j\,\pi / M a} \qquad [\ k_j = \frac{m_j\,\pi}{M a}\ ]$$
$$= \prod_{j=1}^{d} 2 M a\, \delta_{m_j 0}$$

$$= V\,\delta_{\boldsymbol{k}\,0} \tag{A.19}$$

Note that we have used $M\,a$ instead of $(M-1)\,a$ as the upper limit of $d\,x_j$ in order to satisfy

$$\int_V d\,\boldsymbol{x} = V = (2\,M\,a)^d = \prod_{j=1}^{d} \int_{-M\,a}^{M\,a} d\,x_j$$

(A.10) thus becomes

$$S_{\boldsymbol{n}} = \left(\frac{2\,\pi}{a}\right)^d \int_{\text{BZ}} d\,\boldsymbol{k}\, S_{\boldsymbol{k}}\, e^{i\,\boldsymbol{k}\cdot\boldsymbol{n}\,a}$$

$$\to \qquad S(\boldsymbol{x}) = \left(\frac{2\,\pi}{a}\right)^d \int_{\text{BZ}} d\,\boldsymbol{k}\, e^{i\,\boldsymbol{k}\cdot\boldsymbol{x}}\, S(\boldsymbol{k}) \tag{A.20}$$

where $S(\boldsymbol{k}) = S_{\boldsymbol{k}}$ at all discrete $\boldsymbol{k}$ points allowed for $S_{\boldsymbol{k}}$,

$S(\boldsymbol{x})$ is therefore the continuum approximation of $S_{\boldsymbol{n}}$. Note that $S(\boldsymbol{x})$ & $S(\boldsymbol{k})$ are both dimensionless.

n-Ball

The n-D spherical coordinates $(r,\ \phi_1,\ \phi_2,\ \ldots,\ \phi_{n-1})$ are related to the Cartesian coordinates $(x_1,\ x_2,\ \ldots,\ x_n)$ by

$$\begin{aligned}
x_1 &= r\cos\phi_1 \\
x_2 &= r\sin\phi_1\cos\phi_2 \\
x_3 &= r\sin\phi_1\sin\phi_2\cos\phi_3 \\
&\vdots \\
x_{n-1} &= r\sin\phi_1\sin\phi_2\ldots\sin\phi_{n-2}\cos\phi_{n-1} \\
x_n &= r\sin\phi_1\sin\phi_2\ldots\sin\phi_{n-2}\sin\phi_{n-1}
\end{aligned}$$

where

$$0 \le r < \infty, \qquad 0 \le \phi_j < \pi \quad \forall\ j < n-1, \qquad 0 \le \phi_{n-1} < 2\,\pi$$

The volume element is therefore given by

$$\begin{aligned}
d\,V_n &= d\,x_1\,d\,x_2\ldots d\,x_n \\
&= \frac{\partial(x_1,\ \ldots,\ x_n)}{\partial(r,\ \phi_1,\ \ldots,\ \phi_{n-1})}\,d\,r\,d\,\phi_1\ldots d\,\phi_{n-1} \\
&= r^{n-1}\sin^{n-2}\phi_1\sin^{n-3}\phi_2\ldots\sin^2\phi_{n-3}\sin\phi_{n-2}\,d\,r\,d\,\phi_1\ldots d\,\phi_{n-1} \qquad (\text{A.21}) \\
&= r^{n-1}\,d\,r\,d\,\Omega_{n-1}
\end{aligned}$$

where

$$d\,\Omega_{n-1} = \sin^{n-2}\phi_1\sin^{n-3}\phi_2\ldots\sin^2\phi_{n-3}\sin\phi_{n-2}\,d\,\phi_1\ldots d\,\phi_{n-1}$$

and Ω_n is the n-D solid angle.

The surface element of an n-sphere of radius r is

$$d\,S_n = r^n\,d\,\Omega_n$$

Therefore, the volume of an n-ball of radius R is related to its $(n-1)$-sphere surface by

$$\begin{aligned}
V_n(R) &= \int_0^R r^{n-1}\,d\,r \int d\,\Omega_{n-1} = \frac{1}{n}R^n\,\Omega_{n-1} \\
&= \frac{1}{n}R^n\,\frac{1}{R^{n-1}}\,S_{n-1}(R) = \frac{R}{n}\,S_{n-1}(R)
\end{aligned} \tag{A.22}$$

Comparing

$$\Omega_{n-1} = \int_0^\pi \sin^{n-2}\phi_1 \, d\,\phi_1 \int_0^\pi \sin^{n-3}\phi_2 \, d\,\phi_2 \ldots \int_0^\pi \sin\phi_{n-2} \, d\,\phi_{n-2} \int_0^\pi d\,\phi_{n-1}$$

with

$$\Omega_n = \int_0^\pi \sin^{n-1}\phi_1 \, d\,\phi_1 \int_0^\pi \sin^{n-2}\phi_2 \, d\,\phi_2 \ldots \int_0^\pi \sin\phi_{n-1} \, d\,\phi_{n-1} \int_0^\pi d\,\phi_n$$

we have

$$\Omega_n = \Omega_{n-1} \int_0^\pi \sin^{n-1}\phi_1 \, d\,\phi_1$$

$$= \Omega_{n-1} \frac{\sqrt{\pi}\,\Gamma\left(\frac{n}{2}\right)}{\Gamma\left(\frac{n+1}{2}\right)} \qquad \text{[See §Code.]}$$

$$= \Omega_{n-2} \frac{\sqrt{\pi}\,\Gamma\left(\frac{n-1}{2}\right)}{\Gamma\left(\frac{n}{2}\right)} \frac{\sqrt{\pi}\,\Gamma\left(\frac{n}{2}\right)}{\Gamma\left(\frac{n+1}{2}\right)} = \Omega_{n-2} \frac{\pi\,\Gamma\left(\frac{n-1}{2}\right)}{\Gamma\left(\frac{n+1}{2}\right)}$$

$$= \Omega_0\, \pi^{n/2} \frac{\Gamma\left(\frac{1}{2}\right)}{\Gamma\left(\frac{n+1}{2}\right)}$$

$$= \frac{2\,\pi^{(n+1)/2}}{\Gamma\left(\frac{n+1}{2}\right)}$$

where we have used

$$\Omega_0 = 2 \;\; \text{since} \quad V_1 = R\,\Omega_0 = 2\,R$$

Hence,

$$S_n(R) = \frac{2\,\pi^{(n+1)/2}}{\Gamma\left(\frac{n+1}{2}\right)} R^n$$

$$V_n(R) = \frac{2\,\pi^{n/2}}{\Gamma\left(\frac{n}{2}\right)} \frac{1}{n} R^n = \frac{\pi^{n/2}}{\Gamma\left(\frac{n}{2}+1\right)} R^n \qquad \text{(A.23)}$$

Code

```
Assuming[n > 0, ∫_0^π Sin[ϕ]^(n-1) ⅆϕ]
```

$$\frac{\sqrt{\pi}\ \text{Gamma}\left[\frac{n}{2}\right]}{\text{Gamma}\left[\frac{1+n}{2}\right]}$$

```
Assuming[n > 0 && k > 0 && r > 0, ∫_0^∞ ρ Exp[-1/(2 n) (k^2 + r) ρ^2] ⅆρ]
```

$$\frac{n}{k^2 + r}$$

Assuming$\left[n > 0 \,\&\&\, k > 0 \,\&\&\, r > 0,\ \int_0^\infty \rho^3\, \mathrm{Exp}\left[-\frac{1}{2\,n}\left(k^2 + r\right)\rho^2\right] d\rho\right]$

$$\frac{2\,n^2}{\left(k^2 + r\right)^2}$$

$\{\lambda, ev\}$ = **Eigensystem**$\left[\begin{pmatrix} 2 & \frac{24\,d}{(\pi/ap)^2 + r} \\ 0 & 4 - d \end{pmatrix}\right]$

$$\left\{\{2, 4 - d\}, \left\{\{1, 0\}, \left\{-\frac{24\,ap^2\,d}{(-2 + d)\left(\pi^2 + ap^2\,r\right)}, 1\right\}\right\}\right\}$$