In the general case of a random isotropic fractal, the *fractal* or *Hausdorff* dimension d_f is defined via

$$n(r) \sim (r/a)^{d_f}. \tag{2.12.12}$$

This is a generalization of the relation $n \sim r^d$ valid for normal compact objects. The fractal dimension of a polymer is thus $1/\nu$. The pair distribution function and static structure factor for a general fractal are given by

$$\begin{aligned} g_F(r) &\sim n/r^d \sim 1/(a_f^d r^{d-d_f}), \qquad \text{or } \alpha = d - d_f \\ S(q) &\sim (qa)^{-d_f}. \end{aligned} \tag{2.12.13}$$

It is very easy to get a physical feel for what the correlation and scattering functions mean by looking at Figs. 2.12.4 and 2.12.5. Fig. 2.12.4 is an electron micrograph of an aggregate of gold particles formed under highly nonequilibrium conditions. The uniform-size 50Å particles were in stable suspension because of repulsion between the like surface charges. The charges were then chemically removed. The particles diffused until they collided and then stuck wherever they hit. The process is known as *diffusion limited aggregation* (DLA). The mass correlation function was calculated from the electron micrograph by randomly picking a point in the cluster, drawing a circle of radius r and counting the number of particles intersecting the circle. The process was repeated for many origins and many radii. Since the picture is a projection of the structure in two dimensions, it is fractal with $g(r) \sim 1/r^{2-d_f}$, and the log-log plot indicates a slope of 0.25 ($d_f = 1.75 \pm 0.05$) until r approaches the size of the cluster at which point it rapidly decreases.

The same system was studied by both neutron scattering and light scattering. The resulting structure function is shown in Fig. 2.12.5. $S(q)$ should have the form q^{-d_f} until q reaches a crossover value. The $S(q)$ data on this sample give $d_f \sim 1.80$. For higher q the scattering probes distances smaller than a particle size, and the objects no longer look fractal. Fig. 2.12.5 also serves as a good example of the range covered by light ($q \geq 2\pi/\lambda \geq 2\pi/1500$Å) and neutron scattering ($q \geq 2\pi/1$Å).

Appendix 2A Fourier transforms

In this appendix, we will review Fourier transforms for functions of one- and d-dimensional continuous variables and for functions defined at lattice sites on one- and d-dimensional lattices.

1 One dimension

We begin with a function $f(x)$ of a single variable x in the interval $[-L/2, L/2]$ (i.e. $-L/2 \leq x \leq L/2$). If $f(x)$ satisfies reasonable continuity and boundedness conditions (e.g. it does not have an infinite number of zeros in some finite interval of x), it can be expanded in a uniformly convergent Fourier series:

$$f(x) = \sum_q \psi_q(x) f(q) , \tag{2A.1}$$

where $\psi_q(x)$ satisfies the same boundary conditions as $f(x)$. Common boundary conditions on $f(x)$ are $f(x = \pm L/2) = 0$ or $f'(x = \pm L/2) = 0$. In condensed matter physics, one is often interested in bulk systems in the thermodynamic limit, $L \to \infty$, for which most physical properties of interest do not depend on the boundary conditions. In this case, any physically reasonable boundary condition can be imposed. The periodic boundary condition requiring $f(x)$ to be a periodic function of period L,

$$f(x) = f(x + L) , \tag{2A.2}$$

is computationally the simplest and is almost universally used in situations where surface properties are not relevant. The condition (2A.2) is equivalent to wrapping the line of length L on a circle of circumference L and tying the two ends together. The functions $\psi_q(x)$ must satisfy the periodic boundary condition and can be chosen to be

$$\psi_q(x) = Ae^{iqx} , \tag{2A.3}$$

where

$$q = \frac{2\pi}{L} n, \qquad n = 0, \pm 1, \pm 2, ... \tag{2A.4}$$

and where A is an arbitrary normalization constant. The functions e^{iqx} satisfy the *orthogonality condition,*

$$\int_{-L/2}^{L/2} dx e^{i(q-q')x} = \frac{\sin[(q-q')L/2]}{[(q-q')/2]} = L\delta_{n,n'} = L\delta_{q-q',0} , \tag{2A.5}$$

where $\delta_{a,b}$ is the Kronecker delta ($\delta_{a,b} = 1$ if $a = b$ and $\delta_{a,b} = 0$ otherwise) and the *completeness condition,*

$$\sum_q e^{-iqx} = \lim_{N\to\infty} \sum_{N-1}^{N-1} e^{-i(2\pi n/L)x} = \lim_{N\to\infty} \frac{\sin[2\pi(N-1/2)x/L]}{\sin(\pi x/L)} = L\delta(x) , \tag{2A.6}$$

where $\delta(x)$ is the Dirac delta that is zero except at $x = 0$ but whose integral over x is unity. Thus, for periodic boundary conditions,

$$\left.\begin{aligned} f(x) &= A\textstyle\sum_q e^{iqx} f(q), \\ f(q) &= \frac{1}{AL}\int_{-L/2}^{L/2} e^{-iqx} f(x) dx. \end{aligned}\right\} \tag{2A.7}$$

To treat systems in the limit $L \to \infty$, one takes the continuum limit in which $q = (2\pi/L)n$ is treated as a continuous variable and

$$\sum_q \equiv \sum_n \Delta n = \frac{L}{2\pi} \sum_q \Delta q \to L \int_{-\infty}^{\infty} \frac{dq}{2\pi} , \tag{2A.8}$$

where $\Delta n = 1$. Thus Eqs. (2A.7) can be rewritten as

$$f(x) = AL \int_{-\infty}^{\infty} \frac{dq}{2\pi} e^{iqx} f(q) \overset{LA=1}{\to} \int_{-\infty}^{\infty} \frac{dq}{2\pi} e^{iqx} f(q), \tag{2A.9}$$

$$f(q) = \frac{1}{AL} \int_{-\infty}^{\infty} dx e^{-iqx} f(q) \overset{LA=1}{\to} \int_{-\infty}^{\infty} dx e^{-iqx} f(q) . \tag{2A.10}$$

The normalization constant A is often chosen to be equal to L^{-1} so that the factors LA and $(LA)^{-1}$ become unity as shown in the final form on the right hand side of Eqs. (2A.9) and (2A.10). Other choices, such as $A = L^{-1/2}$ so that $L^{-1/2}$ appears as a factor in both Eqs. (2A.9) and (2A.10), are also used. In the continuum limit, the orthogonality and completeness relations (2A.5) and (2A.6) become

$$\int_{-\infty}^{\infty} dx e^{i(q-q')x} = \lim_{L\to\infty} L\delta_{q-q',0} \equiv 2\pi\delta(q-q') \tag{2A.11}$$

and

$$\int_{-\infty}^{\infty} \frac{dq}{2\pi} e^{-iq(x-x')} = \delta(x-x'). \tag{2A.12}$$

The identification of $L\delta_{q,q'}$ with $2\pi\delta(q-q')$ can be seen from

$$\sum_q \delta_{q,0} = 1 = \frac{L}{2\pi}\int dq\delta_{q,0} \to \int_{-\infty}^{\infty} dq\delta(q)\,. \tag{2A.13}$$

2 d dimensions

The generalization of the above formulae to d dimensions is straightforward. Let $f(\mathbf{x})$ be a function of a d-component vector $\mathbf{x} = (x_1, x_2, ..., x_d)$ and impose periodic boundary conditions on each of the components of $\mathbf{x}$:

$$f(x_1, ..., x_i, ..., x_d) = f(x_1, ..., x_i + L_i, ..., x_d)\,, \qquad i = 1, 2, ..., d\,. \tag{2A.14}$$

Then $f(\mathbf{x})$ can be expanded in a Fourier series similar to Eqs. (2A.7):

$$f(\mathbf{x}) \;=\; A\sum_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{x}} f(\mathbf{q}) \tag{2A.15}$$

$$f(\mathbf{q}) \;=\; \frac{1}{AV}\int d^d x e^{-i\mathbf{q}\cdot\mathbf{x}} f(\mathbf{x})\,, \tag{2A.16}$$

where $V = L_1 L_2 ... L_d$ and

$$\mathbf{q} = \left(\frac{2\pi}{L_1}n_1, \frac{2\pi}{L_2}n_2, ..., \frac{2\pi}{L_d}n_d\right)\,, \tag{2A.17}$$

where the coefficients n_i are integers. In the infinite volume limit, these relations become

$$\begin{aligned} f(\mathbf{x}) \;&=\; A\sum_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{x}} f(\mathbf{q}) = AV\int \frac{d^d q}{(2\pi)^d} e^{i\mathbf{q}\cdot\mathbf{x}} f(\mathbf{q}) \\ &\overset{AV=1}{\rightarrow}\; \int \frac{d^d q}{(2\pi)^d} e^{i\mathbf{q}\cdot\mathbf{x}} f(\mathbf{q}) \end{aligned} \tag{2A.18}$$

$$f(\mathbf{q}) \;=\; \frac{1}{AV}\int d^d x e^{-i\mathbf{q}\cdot\mathbf{x}} f(\mathbf{x}) \overset{AV=1}{\rightarrow} \int d^d x e^{-i\mathbf{q}\cdot\mathbf{x}} f(\mathbf{x}), \tag{2A.19}$$

where again the normalization factor A is often chosen to be equal to V^{-1} as indicated by the final form of these equations. It is understood that the $\mathbf{x}$- and $\mathbf{q}$-integrals in Eqs. (2A.18) and (2A.19) are over all space. Finally, in the infinite volume, continuum limit, the orthogonality and completeness conditions become

$$\int d^d x e^{i(\mathbf{q}-\mathbf{q}')\cdot\mathbf{x}} = V\delta_{\mathbf{q},\mathbf{q}'} = (2\pi)^d \delta^{(d)}(\mathbf{q}-\mathbf{q}') \tag{2A.20}$$

and

$$\int \frac{d^d q}{(2\pi)^d} e^{-i\mathbf{q}\cdot(\mathbf{x}-\mathbf{x}')} = \delta^{(d)}(\mathbf{x}-\mathbf{x}')\,, \tag{2A.21}$$

where $\delta^{(d)}(\mathbf{x})$ is a d-dimensional Dirac delta function.

3 Transforms on a lattice

Often one is interested in functions that are defined only at points on a regular periodic lattice rather than at all points in space. The Fourier transformation of these functions is the subject of this sub-section.

One-dimensional lattices Let f_l be a function of the integer l indexing the lattice site located at position $R_l = la$ of a one-dimensional lattice with lattice spacing a (see Sec. 2.5). The function f_l can be expanded in a discrete Fourier series

$$f_l = \sum_q \tilde{\varphi}_q(l) f_q, \tag{2A.22}$$

where $\tilde{\varphi}_q(l)$ satisfies the same boundary conditions as f_l. Again, we choose the periodic boundary condition,

$$f_l = f_{l+N}, \tag{2A.23}$$

where N is an integer. In this case, we can choose

$$\tilde{\varphi}_q(l) = Ae^{iqR_l} = \tilde{\varphi}_q(l+N)\,, \tag{2A.24}$$

where

$$q = \frac{2\pi}{Na}n, \tag{2A.25}$$

where n is an integer. Because R_l is an integral multiple of the lattice spacing a, the function $\tilde{\varphi}_q(x)$ in Eq. (2A.23) is periodic in q as well as in l:

$$\tilde{\varphi}_q(l) = \tilde{\varphi}_{q+(2\pi)/a}\,(l). \tag{2A.26}$$

Thus all the functions $\tilde{\varphi}_q(l)$ and $f(q)$ are completely characterized by q in the interval $[-\pi/a, \pi/a]$, i.e., by q in the first *Brillouin zone* (BZ) of the one-dimensional lattice.

The number of points in the first BZ is equal to the number of sites N in the direct lattice. This follows because the number of points in some region of space is equal to its "volume" divided by the "volume" per point. The volume of the first BZ of a one-dimensional lattice is $2\pi/a$ and volume per point is simply $\Delta q = (2\pi)/Na$, so that

$$\text{number of points in first BZ} = \frac{2\pi}{a}\frac{1}{\Delta q} = \frac{2\pi/a}{(2\pi)/Na} = N. \tag{2A.27}$$

The functions e^{iqR_l} satisfy an orthogonality condition similar to that of the functions e^{iqx}:

$$\sum_{l=0}^{N} e^{i(q-q')R_l} = N\delta_{q,q'} \overset{N\to\infty}{\to} \frac{2\pi}{a}\delta(q-q'), \tag{2A.28}$$

where Eq. (2A.11) with $L = Na$ was used to relate the Kronecker delta to the Dirac delta. The completeness condition is

$$\sum_{q\in 1\text{st BZ}} e^{iqR_l} = \frac{1-e^{iNl}}{1-e^{il}} = N\delta_{l,0}. \tag{2A.29}$$

In the continuum limit, this equation becomes

$$a\int_{-\pi/a}^{\pi/a} \frac{dq}{2\pi} e^{iqR_l} = \delta_{l,0}. \tag{2A.30}$$

When the above results are combined, the lattice Fourier transforms can be written as

$$f_l \quad = \quad A \sum_{q\in 1\text{st BZ}} e^{iqR_l} f_q \overset{N\to\infty}{\to} A(Na)\int_{-\pi/a}^{\pi/a} \frac{dq}{2\pi} e^{iqR_l} f_q$$

$$\stackrel{ANa=1}{\rightarrow} \int_{-\pi/a}^{\pi/a} \frac{dq}{2\pi} e^{iqR_l} f_q \tag{2A.31}$$

$$f_q = \frac{1}{NA} \sum_l e^{-iqR_l} f_l \stackrel{ANa=1}{\rightarrow} a \sum_l e^{-iqR_l} f_l. \tag{2A.32}$$

Again, the choice of A is arbitrary. Often the choice $A = (1/Na)$ is made as shown on the far right hand side of these equations. In this case, $(NA)^{-1} = a$, and the sum over l in Eq. (2A.32) could be replaced by an integral over R_l in a spatial continuum limit.

d-dimensional lattices The generalization of lattice Fourier transforms to d-dimensional lattices is again straightforward. If $f_{\mathbf{l}}$ is a function of the lattice index $\mathbf{l}$ satisfying periodic boundary conditions, $f_{\mathbf{l}} = f_{\mathbf{l}+\mathbf{N}}$, where $\mathbf{N} = (N_1, N_2, ..., N_d)$, then

$$f_{\mathbf{l}} = \sum_{\mathbf{q}} \tilde{\psi}_{\mathbf{q}}(\mathbf{l}) f_{\mathbf{q}}, \tag{2A.33}$$

where, since $\mathbf{R}_{\mathbf{l}+\mathbf{N}} = \mathbf{R}_{\mathbf{l}} + \mathbf{R}_{\mathbf{N}}$,

$$\tilde{\psi}_{\mathbf{q}}(\mathbf{l}) = A e^{i\mathbf{q}\cdot\mathbf{R}_{\mathbf{l}}} \tag{2A.34}$$

with

$$\mathbf{q} = \left(\frac{2\pi}{N_1 a} n_1, \frac{2\pi}{N_2 a} n_2, ..., \frac{2\pi}{N_d a} n_d \right) . \tag{2A.35}$$

The restriction of $\mathbf{R}_{\mathbf{l}}$ to lattice points leads to

$$\tilde{\psi}_{\mathbf{q}+\mathbf{G}}(\mathbf{l}) = \tilde{\psi}_{\mathbf{q}}(\mathbf{l}) , \tag{2A.36}$$

where $\mathbf{G}$ is a reciprocal lattice vector. Thus, as in the one-dimensional case, only wave vectors $\mathbf{q}$ in the first Brillouin zone need be considered. The number of points in the first Brillouin zone is again equal to the number of points, $N = N_1 N_2 ... N_d$ in the lattice. The orthogonality and completeness conditions are now

$$v_0 \sum_{\mathbf{l}} e^{i(\mathbf{q}-\mathbf{q}')\cdot\mathbf{R}_{\mathbf{l}}} = V \delta_{\mathbf{q},\mathbf{q}'} = (2\pi)^d \delta^{(d)}(\mathbf{q} - \mathbf{q}'), \tag{2A.37}$$

and

$$\frac{1}{N} \sum_{\mathbf{q}} e^{-i\mathbf{q}\cdot(\mathbf{R}_{\mathbf{l}}-\mathbf{R}_{\mathbf{l}'})} \rightarrow v_0 \int \frac{d^d q}{(2\pi)^d} e^{-i\mathbf{q}\cdot(\mathbf{R}_{\mathbf{l}}-\mathbf{R}_{\mathbf{l}'})} = \delta_{\mathbf{l},\mathbf{l}'}, \tag{2A.38}$$

where $v_0 = V/N$ is the volume of a unit cell and the q-integral is over the first BZ. The Fourier transform equations are

$$f_{\mathbf{l}} = A \sum_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{R}_{\mathbf{l}}} f_{\mathbf{q}} \rightarrow AV \int \frac{d^d q}{(2\pi)^d} e^{i\mathbf{q}\cdot\mathbf{R}_{\mathbf{l}}} f_{\mathbf{q}}$$

$$\stackrel{AV=1}{\rightarrow} \int \frac{d^d q}{(2\pi)^d} e^{i\mathbf{q}\cdot\mathbf{R}_{\mathbf{l}}} \tag{2A.39}$$

and

$$f_{\mathbf{q}} = \frac{1}{NA} \sum_{\mathbf{l}} e^{-i\mathbf{q}\cdot\mathbf{R}_{\mathbf{l}}} f_{\mathbf{l}} \stackrel{AV=1}{\rightarrow} v_0 \sum_{\mathbf{l}} e^{-i\mathbf{q}\cdot\mathbf{R}_{\mathbf{l}}} . \tag{2A.40}$$

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