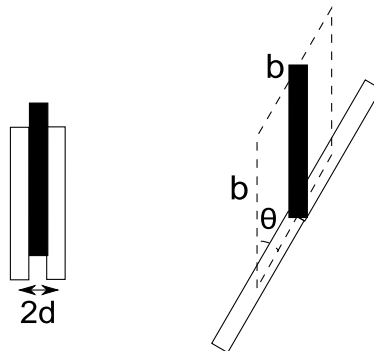


1.9. Solutions to Problem Set 1

- Fixed angle θ between rods:* Imagine infinite straight lines passing through the rods axes. The rods will have a chance at colliding only if the shortest distance between these lines is smaller than rod diameter d (see left panel in the figure). Furthermore, for collisions, the position of the center of one rod with respect to the other has to be in the area outlined by the dashed line in the drawing (right panel), when looked in the plane parallel to the axes of both rods. Thus the excluded volume is just a product of the excluded area of the parallelogram in the figure and of $2d$ (see figure):

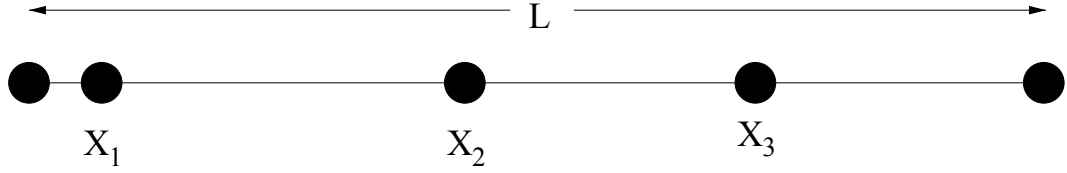
$$v(\theta) = 2db^2 \sin \theta. \quad (1.61)$$



- For random angles,* we just average the result of the previous question over all spatial angles. Notice that θ changes in $[0, \pi/2]$ range (see Fig.) and so the range of the spatial angles is 2π :

$$v = \frac{1}{2\pi} \int_0^{2\pi} d\phi \int_0^{\pi/2} v(\theta) \sin \theta d\theta = 2 \int_0^{\pi/2} \sin^2 \theta d\theta = \frac{\pi}{2} db^2. \quad (1.62)$$

- As long as the spheres do not collide the total energy of this system is constant (zero) and we can treat this system as a part of microcanonical ensemble. Thus any allowed state of the system (i.e. configuration of the beads without collisions) has equal probability.



The total amount of configurations (degeneracy of the system, which in this case is equivalent to the partition function Z (why?)) can be calculated as follows:

$$Z = \int_{\sigma}^{L-3\sigma} dX_1 \int_{X_1+\sigma}^{L-2\sigma} dX_2 \int_{X_2+\sigma}^{L-\sigma} dX_3 = \frac{(L-4\sigma)^3}{6} \quad (1.63)$$

The probability density $P(X)$ of finding a system in a configuration with a bead at coordinate X (defined so that probability of finding a bead in $[X, X + dX]$ range is $dp(X) = P(X)dX$) is proportional to the number of microstates $\mathcal{N}(X)$ of the system with a bead at X :

$$P(X) = \frac{\mathcal{N}(X)}{Z} \quad (1.64)$$

We will split the range of possible X values into three subranges: a) $[\sigma, 2\sigma]$, b) $[2\sigma, 3\sigma]$, c) $[3\sigma, L - 3\sigma]$. There are two additional cases around the right edge of the system (guess which) which are symmetric to cases (a) and (b).

Let's call a bead at X a *probe*.

a) $[\sigma, 2\sigma]$: in this case, no beads can fit into the space between the left edge of the system and the probe. Thus the two remaining free beads have to fit into the $[X + \sigma, L - \sigma]$ space:

$$P(X) = \frac{\mathcal{N}(X)}{Z} = \frac{1}{Z} \int_{X_1+\sigma}^{L-2\sigma} dX_2 \int_{X_2+\sigma}^{L-\sigma} dX_3 = \frac{1}{Z} \frac{(L - X - 3\sigma)^2}{2} \quad (1.65)$$

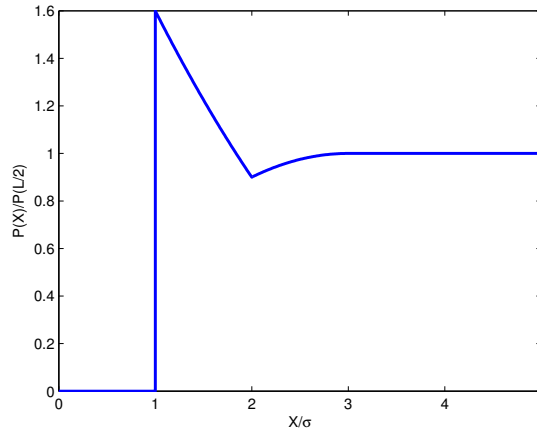
b) $[2\sigma, 3\sigma]$: in this case one bead can fit into the space between left edge of the system and the probe. The total number of microstates is combined of the number of states with two beads to the right of the probe as in the case (a) and of the number of states with one bead to the left and one bead to the right of the probe:

$$\begin{aligned} P(X) = \frac{\mathcal{N}(X)}{Z} &= \frac{1}{Z} \left[\frac{(L - X - 3\sigma)^2}{2} + (X - 2\sigma)(L - X - 2\sigma) \right] = \\ &= \frac{1}{Z} \left[-\frac{X^2}{2} + 3\sigma X + \frac{L^2}{2} - 5L\sigma + \frac{17}{2}\sigma^2 \right] \end{aligned} \quad (1.66)$$

- c) $[3\sigma, L-3\sigma]$: in this case both free beads can fit anywhere. We can use the expression from (b) with another term added which takes into account the states with two beads in between the left edge of the system and the probe:

$$P(X) = \frac{1}{Z} \left[\frac{(L - X - 3\sigma)^2}{2} + (X - 2\sigma)(L - X - 2\sigma) + \frac{(X - 3\sigma)^2}{2} \right] =$$

$$= \frac{1}{Z} \left[\frac{L^2}{2} - 5L\sigma + 13\sigma^2 \right] \quad (1.67)$$



Notice that:

- The probability density to find a bead and the average density of the beads is the same thing, just think how you would define both;
- At the limits of each range the corresponding expressions give the same numbers (check!!!): the overall function is continuous in this sense (but not its derivative)
- The $P(X)$ function arrives at a constant value for $3\sigma < X < L - 3\sigma$
- The $P(X)$ is drawn schematically for $L = 8\sigma$. For the drawing $P(X)$ is normalized by its constant value in $3\sigma < X < L - 3\sigma$ range and the coordinate is normalized by the bead diameter. Notice the presence of one maximum and one minimum in the function $P(X)$.

3. The second virial coefficient is $a = \int (1 - e^{-\beta u(r)}) d\vec{r}$.

For potential

$$u(r) = \begin{cases} -\psi(r), & r < \sigma \\ \infty, & r > \sigma \end{cases} \quad (1.68)$$

we get

$$\begin{aligned} a &= \int (1 - e^{-\beta u(r)}) d\vec{r} = 4\pi \int_0^\sigma r^2 dr + 4\pi \int_\sigma^\infty (1 - e^{-\frac{\psi}{\tau}}) r^2 dr = \\ &= \frac{4\pi}{3} \sigma^3 + 4\pi \cdot \frac{1}{\tau} \int_\sigma^\infty \psi(r) r^2 dr = 4\pi \left(\frac{\sigma^3}{3} - \frac{I}{\tau} \right) \end{aligned} \quad (1.69)$$

when $I \equiv \int_\sigma^\infty \psi(r) r^2 dr$. The integral is converging assuming $\psi(r)$ decays to zero at infinity much faster than r^2 diverges.

The second virial coefficient is zero when $\tau = \frac{3I}{\sigma^3}$. At this temperature the gas behaves almost as an ideal gas.

4. Using the definition of ensemble average we write:

$$\frac{\langle U \rangle}{N} = \frac{1}{N} \cdot \frac{1}{N!(2\pi\hbar)^{3N}} \int U(\{\vec{p}_i, \vec{r}_i\}_N) P(\{\vec{p}_i, \vec{r}_i\}_N) d\vec{p}_1 d\vec{r}_1 \dots d\vec{p}_N d\vec{r}_N$$

We substitute $U = \frac{1}{2} \sum_{i \neq j} u(r_{ij})$ and get

$$\frac{\langle U \rangle}{N} = \frac{1}{N} \cdot \frac{1}{N!(2\pi\hbar)^{3N}} \frac{1}{2} \sum_{i \neq j} \int u(|r_i - r_j|) P(\{\vec{p}_i, \vec{r}_i\}_N) d\vec{p}_1 d\vec{r}_1 \dots d\vec{p}_N d\vec{r}_N.$$

Since molecules are indistinguishable the expression is symmetric in r_i and all of the terms in the sum over i and j are equivalent. Thus only one term, say corresponding to $i=1, j=2$ can be calculated, and then multiplied by the number of terms $N(N-1)$. The probability $P(\vec{p}_i, \vec{r}_i)$ is given by Eq. 1.19 and Eq. 1.18

$$P(\vec{p}_i, \vec{r}_i) = \frac{e^{-\beta(\sum \frac{p_i^2}{2m} + U(\vec{r}_1 \dots \vec{r}_N))}}{Z_N} = \frac{N! e^{-\beta(\sum \frac{p_i^2}{2m} + U(\vec{r}_1 \dots \vec{r}_N))}}{n_q^{3N} Q_N}.$$

Then substituting the expression for probability density and integrating over momenta we have

$$\begin{aligned} \frac{\langle U \rangle}{N} &= \frac{1}{2N} \cdot \frac{N(N-1)}{(2\pi\hbar)^{3N}} \cdot \frac{\int u(|r_1 - r_2|) e^{-\beta(\sum \frac{p_i^2}{2m} + U(\vec{r}_1 \dots \vec{r}_N))} d\vec{p}_1 d\vec{r}_1 \dots d\vec{p}_N d\vec{r}_N}{n_q^{3N} Q_N} \\ &= \frac{N(N-1)}{2N} \cdot \frac{\int u(|r_1 - r_2|) e^{-\beta U(\vec{r}_1 \dots \vec{r}_N)} d\vec{r}_1 \dots d\vec{r}_N}{Q_N} \end{aligned}$$

We now use the definition Eq. 1.37

$$n^2 g^{(2)}(\vec{r}_1, \vec{r}_2) = \frac{N(N-1)}{Q_N} \int d\vec{r}_3 d\vec{r}_4, \dots, d\vec{r}_N e^{-\beta U(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N)}$$

$$\begin{aligned} \frac{\langle U \rangle}{N} &= \frac{n^2}{2N} \int g^{(2)}(|\vec{r}_1 - \vec{r}_2|) \cdot u(|\vec{r}_1 - \vec{r}_2|) d\vec{r}_1 d\vec{r}_2 = \\ &= \frac{n^2}{2N} \int g(|\vec{r}|) \cdot u(|\vec{r}|) d\vec{r} d\vec{r}_2 = \frac{V}{2} \cdot \frac{1}{N} n^2 \int u(r) g(r) d\vec{r}, \end{aligned}$$

where we changed to $\vec{r} = \vec{r}_1 - \vec{r}_2$ variable and performed integration over \vec{r}_2 (which gave us V). Then

$$\frac{\langle U \rangle}{N} = \frac{n}{2} \int u(r) g(r) d\vec{r} = 2\pi n \int u(r) g(r) r^2 dr$$

The average energy per molecule is the interaction energy $u(r)$ of two particles, multiplied by the density $ng(r)$ of molecules at distance r from the "test" molecule and summing over r . The result is divided by two so every pair of particles is counted only once.

5. • We assume that the system is ergodic and change time averaged values by ensemble averaged values i.e. for an ergodic system the statement $\bar{\mathcal{V}} = -2\bar{K}$ is equivalent to $\langle \mathcal{V} \rangle = -2\langle K \rangle$.

From equipartition we know that $\langle K \rangle = (3/2)Nk_B T$

We split the forces into internal to the system and external. For internal forces we can write

$$\vec{F}_i^{int} = -\frac{\partial}{\partial \vec{r}_i} U(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N)$$

We assume that external forces are short-ranged (as all of the other molecular forces) and act only through the bounding surface S of the system. Then

$$\langle \mathcal{V}^{ext} \rangle = \left\langle \sum \vec{r}_i \vec{F}_i^{ext} \right\rangle = - \int_S \vec{r} p d\vec{S} = -p \int_V \nabla \vec{r} d\vec{r} = -3p \int_V d\vec{r} = -3pV,$$

where we made use of the Gauss theorem relating flux through the surface to divergence. Minus sign stems from the fact that the external pressure acts inward into the system while $d\vec{S}$ is usually defined outward. An interesting question is why we assume pressure only, i.e. no tangential forces acting on the system boundary: in thermal equilibrium one does not expect any tangential forces (on average of course). Think why.

Finally, placing it altogether:

$$\langle \mathcal{V} \rangle = \langle \mathcal{V}^{ext} \rangle + \langle \mathcal{V}^{int} \rangle = -3pV - \left\langle \sum_{i=1}^N \vec{r}_i \frac{\partial}{\partial \vec{r}_i} U(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N) \right\rangle = -2\langle K \rangle = -3Nk_B T,$$

or

$$\frac{pV}{Nk_B T} = 1 - \frac{1}{3Nk_B T} \left\langle \sum_{i=1}^N \vec{r}_i \frac{\partial}{\partial \vec{r}_i} U(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N) \right\rangle$$

- The derivation goes exactly as in Problem 4, we just couple symmetric terms:

$$\begin{aligned} & \left\langle \sum_{i=1}^N \vec{r}_i \frac{\partial}{\partial \vec{r}_i} U(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N) \right\rangle = \frac{N(N-1)}{2} \left\langle \vec{r}_1 \frac{\partial}{\partial \vec{r}_1} u(|\vec{r}_1 - \vec{r}_2|) + \vec{r}_2 \frac{\partial}{\partial \vec{r}_2} u(|\vec{r}_2 - \vec{r}_1|) \right\rangle = \\ & = [\vec{r} = \vec{r}_1 - \vec{r}_2] = \frac{N(N-1)}{2} \left\langle \vec{r}_1 \frac{\partial}{\partial \vec{r}} u(|\vec{r}|) - \vec{r}_2 \frac{\partial}{\partial \vec{r}} u(|\vec{r}|) \right\rangle = \frac{N(N-1)}{2} \left\langle \vec{r} \frac{\partial}{\partial \vec{r}} u(|\vec{r}|) \right\rangle = \\ & = \frac{N(N-1)}{2Q_N} \int (\vec{r}_1 - \vec{r}_2) \frac{\partial u(\vec{r}_1 - \vec{r}_2)}{\partial (\vec{r}_1 - \vec{r}_2)} e^{-\beta U(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N)} d\vec{r}_1 d\vec{r}_2, \dots, d\vec{r}_N = \\ & = \frac{n^2}{2} \int (\vec{r}_1 - \vec{r}_2) \frac{\partial u(\vec{r}_1 - \vec{r}_2)}{\partial (\vec{r}_1 - \vec{r}_2)} g^{(2)}(\vec{r}_1 - \vec{r}_2) d\vec{r}_1 d\vec{r}_2 = \frac{n^2 V}{2} \int \vec{r} \frac{du(\vec{r})}{d\vec{r}} g(\vec{r}) d\vec{r} = \\ & = 2\pi n N \int r^3 \frac{du}{dr} g(r) dr \end{aligned}$$

Just substitute this in the result of the previous question to obtain the required relation.

- For low densities $U \approx 0$ for the most of the $\{\vec{r}_1, \dots, \vec{r}_N\}$ space. Then $\int \exp(-\beta U) d\vec{r}_i \approx V$ and respectively $Q_N \approx V^N$. Then from the definition:

$$\begin{aligned} n^2 g^{(2)}(\vec{r}_1, \vec{r}_2) &= \frac{N(N-1)}{Q_N} \int d\vec{r}_3 d\vec{r}_4, \dots, d\vec{r}_N e^{-\beta U(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N)} = \\ &= \frac{N(N-1)}{Q_N} e^{-\beta u(\vec{r}_1 - \vec{r}_2)} \int d\vec{r}_3 d\vec{r}_4, \dots, d\vec{r}_N \exp \left(-\beta \sum_{(i,j) \neq (1,2)} u(\vec{r}_i - \vec{r}_j) \right) = \\ &\approx \frac{N(N-1)}{V^N} e^{-\beta u(\vec{r}_1 - \vec{r}_2)} \cdot V^{N-2} = n^2 e^{-\beta u(\vec{r}_1 - \vec{r}_2)} \end{aligned}$$

Thus $g(r) = e^{-\beta u(r)}$ for low densities. Substitute this into the virial theorem expression Eq. 1.57 (proven in the previous question) and integrate by parts:

$$\begin{aligned} \frac{p}{nk_B T} &= 1 - \frac{2\pi n \beta}{3} \int_0^\infty e^{-\beta u(r)} \frac{du}{dr} r^3 dr = 1 - \frac{2\pi n}{3} \int_0^\infty r^3 d(1 - e^{-\beta u(r)}) = \\ &= 1 - \frac{2\pi n}{3} r^3 (1 - e^{-\beta u(r)}) \Big|_{r=0, \text{exp} \rightarrow 0}^{r \rightarrow \infty, \text{exp} \rightarrow 1} + 2\pi n \int_0^\infty (1 - e^{-\beta u(r)}) r^2 dr = \\ &= 1 + \frac{1}{2} an, \end{aligned}$$

where a is defined in Eq. 1.24.

- The problem of using Eq. 1.57 $u(r)$ is not continuous for hard core potential and as a result $g(r)$ is not continuous either. Remembering, however, that at least for

low densities $g(r) \approx e^{-\beta u(r)}$, we can expect that the function $y(r) = g(r)e^{\beta u(r)}$ is "more" continuous than $g(r)$. Then in terms of $y(r)$ Eq. 1.57 looks like this:

$$\frac{p}{nk_B T} = 1 - \frac{2\pi n}{3k_B T} \int_0^\infty y(r) e^{-\beta u(r)} \frac{du}{dr} r^3 dr = 1 + \frac{2\pi n}{3} \int_0^\infty y(r) \frac{de^{-\beta u(r)}}{dr} r^3 dr$$

Notice now that for a hard core potential Eq. 1.25 the exponent $e^{-\beta u(r)}$ is in fact a Heaviside function switching from zero to 1 at $r = \sigma$. Its derivative is therefore Dirac δ -function $\delta(r - \sigma)$. Then

$$\frac{p}{nk_B T} = 1 + \frac{2\pi n}{3} y(\sigma) \sigma^3$$

Noticing that $y(\sigma + \varepsilon) = g(\sigma + \varepsilon)e^{\beta u(\sigma + \varepsilon)} = g(\sigma + \varepsilon)$, we rewrite the above equation (by the way what is the value of $g(\sigma - \varepsilon)$):

$$\frac{p}{nk_B T} = 1 + \frac{2\pi n}{3} g(\sigma) = 1 + 4\phi g(\sigma)$$

To check this expression at low densities recall that for low densities $g(r) \approx e^{-\beta u(r)}$, i.e. $g(\sigma) \approx 1$ for hard cores in that case.

6. We associate crystals with ordered positioning of atoms (molecules) so that, e.g. in an X-ray experiment scattering from different atoms would add up constructively/destructively at some particular angles and the characteristic Bragg diffraction pattern would be created. For that, the $k - th$ neighbor of any atom should be positioned at the ka distance from the atom, where a is a lattice parameter. We can tolerate small thermal fluctuations around the average position, but not the fluctuations that would diverge with k . Otherwise, no constructive/destructive interference for us.

In the 1D Frenkel model we derived that the probability density of distance distribution for $k + 1$ neighbor is given just by Poisson distribution:

$$P_{k+1}(x) = \frac{(nx)^k}{k!} e^{-nx} n, \quad (1.70)$$

where $x = X - (k + 1)d$ is the "rescaled" coordinate (the real coordinate X from which all of the "dead" space occupied by beads has been subtracted), and $n = \frac{N}{L - Nd}$ is respectively a rescaled density (i.e. the total number of beads N divided by the

overall length of the system L from which the "dead" space has been subtracted).

Then average x_{k+1} and its variance are:

$$\langle x_{k+1} \rangle = \int_0^\infty x \frac{(nx)^k}{k!} e^{-nx} n dx \quad (1.71)$$

$$\langle x_{k+1}^2 \rangle = \int_0^\infty x^2 \frac{(nx)^k}{k!} e^{-nx} n dx \quad (1.72)$$

We solve these with the timeless trick, define:

$$I(\beta) = \int_0^\infty \frac{(nx)^k}{k!} e^{-\beta nx} n dx = \frac{1}{\beta^{k+1}} \underbrace{\int_0^\infty \frac{(\beta nx)^k}{k!} e^{-\beta nx} \beta n dx}_{\text{normalization of Poisson distribution}} = \frac{1}{\beta^{k+1}}. \quad (1.73)$$

Then

$$\langle x_{k+1} \rangle = -\frac{1}{n} \frac{\partial I}{\partial \beta} \Big|_{\beta=1} = -\frac{1}{n} \frac{\partial}{\partial \beta} \left(\frac{1}{\beta^{k+1}} \right) \Big|_{\beta=1} = \frac{k+1}{n} \quad (1.74)$$

$$\langle x_{k+1}^2 \rangle = \frac{1}{n^2} \frac{\partial^2 I}{\partial \beta^2} \Big|_{\beta=1} = \frac{1}{n^2} \frac{\partial^2}{\partial \beta^2} \left(\frac{1}{\beta^{k+1}} \right) \Big|_{\beta=1} = \frac{(k+1)(k+2)}{n^2} \quad (1.75)$$

Switching to k -th neighbor for brevity (i.e. replacing $k+1$ with k everywhere) and moving to real coordinate X , we have for its average and standard deviation:

$$\begin{aligned} \langle X_k \rangle &= \frac{k(L - Nd)}{N} + kd = (L/N)k = ak \\ \sigma_{X_k} &= \sqrt{\langle x_k^2 \rangle - \langle x_k \rangle^2} = \sqrt{\frac{k(k+1)}{n^2} - \frac{k^2}{n^2}} = \frac{\sqrt{k}}{n} = \frac{\sqrt{k}(L - Nd)}{N} = \sqrt{k}(a - d) \end{aligned} \quad (1.76)$$

where $a = L/N$ is the average spacing between beads (equivalent of the lattice parameter).

Thus we see that the distance fluctuations between k -th neighbors diverge with k and the relative positions of the neighbors become poorly defined. The tighter the beads are placed the closer is a to d and smaller the fluctuations. However, for any packing fraction smaller than 1, the fluctuations would diverge with k .

7. Before calculating the structure factor of a sphere, let's derive first the Fourier transform of any spherically symmetric function $f(r)$. We expect its Fourier transform to be spherically symmetric as well and depend on the size (but not direction) of \vec{q} . Without loss of generality, we can align \vec{q} then with Z-axis and use spherical coordinates

(r, θ, ϕ) to integrate over \vec{r} :

$$\begin{aligned}\tilde{f}(q) &= \frac{1}{(2\pi)^{3/2}} \int f(\vec{r}) e^{-i\vec{q}\vec{r}} d\vec{r} = \frac{1}{(2\pi)^{3/2}} \int_0^\infty r^2 dr \int_0^{2\pi} d\phi \int_0^\pi \sin\theta d\theta f(r) e^{-iqr \cos\theta} = \\ &= \frac{1}{(2\pi)^{1/2}} \int_0^\infty r dr f(r) \frac{(e^{iqr} - e^{-iqr})}{iq} = \sqrt{\frac{2}{\pi}} \int_0^\infty r dr f(r) \frac{\sin(qr)}{q}\end{aligned}\quad (1.77)$$

We can now substitute the density of the uniform sphere: $n(r) = n, r < R; n(r) = 0, r > R$:

$$\tilde{n}(q) = \sqrt{\frac{2}{\pi}} \frac{n}{q} \int_0^R r \sin(qr) dr = \sqrt{\frac{2}{\pi}} n \frac{\sin(qR) - qR \cos(qR)}{q^3}.\quad (1.78)$$

Then the structure factor is:

$$S(q) = \frac{\tilde{n}(\vec{q})\tilde{n}(-\vec{q})}{N} = \frac{2}{\pi} n^2 \frac{(\sin(qR) - qR \cos(qR))^2}{q^6 (4/3)n\pi R^3} = \frac{9}{8\pi^3} N \frac{(\sin(qR) - qR \cos(qR))^2}{(qR)^6}\quad (1.79)$$

The prefactor might depend on the precise definition of $S(q)$ and of the Fourier transform. The dependence on q is in the last term in the product.

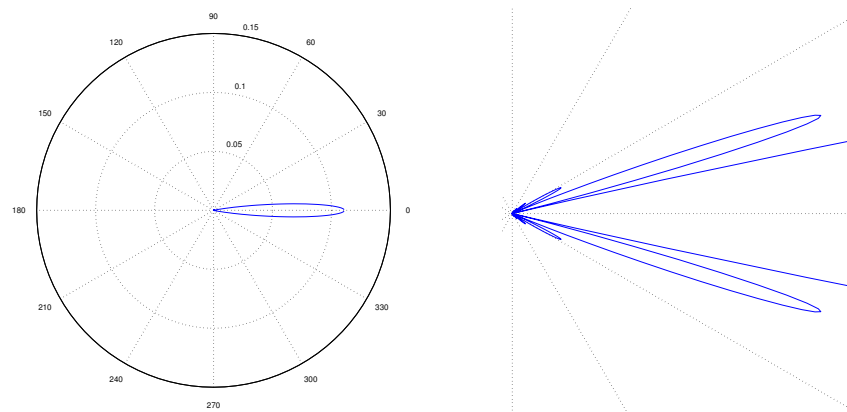
One should remember that \vec{q} is the difference in wave vectors of the incident and scattered light: $\vec{q} = \vec{k}_i - \vec{k}_f$. Since we consider elastic scattering here $k_i = k_f = 2\pi/\lambda$. Then solving a simple triangle of the three vectors we get: $q = (4\pi/\lambda) \sin(\theta/2)$, where θ is the angle between incident and scattered light.

For small particles $\lambda \gg R$, or $qR \ll 1$, We can expand the expression in Taylor series:

$$S(q) \approx \frac{9}{8\pi^3} N \frac{(qR - (qR)^3/6 - qR(1 - (qR)^2)/2)^2}{(qR)^6} = \frac{3}{8\pi^3} N,\quad (1.80)$$

i.e. scattering is uniform, does not depend on direction. This is Rayleigh scattering regime.

For $qR \sim 1$ there will be constructive/destructive interference in different directions (Mie scattering). However the strongest scattering will always be in the direction of $\vec{q} = 0$, i.e. forward scattering. That's why the dust on car windshields limits our vision severely when the sun is roughly in front of us. Showing below the polar plot of scattering for $R = 3\lambda$. There is a dominating peak in the forward scattering but if one zooms in many more smaller peaks show up.



Here is the corresponding Matlab code:

```
theta = (0.001:0.001:0.999)*2*pi;
R = 3; % in terms of wave length
qR = 4*pi*sin(theta/2)*R;
S = (sin(qR) - qR.*cos(qR)).^2./qR.^6;
subplot(1, 2, 1)
polar(theta, S);
subplot(1, 2, 2)
polar(theta, S);
axis(1.0e-03*[-0.0257    0.8755   -0.5100    0.5264])
figure(gcf)
```