

1 Sanity check

The static structure factor is the Fourier transform of the radial distribution function $g_2(r)$.

$$S(\vec{q}) = 1 + \rho \int_V d\vec{r} e^{-i\vec{q}\cdot\vec{r}} g_2(r) \quad (1)$$

r is the distance between two water molecules and \vec{r} is the vector connecting them. To compute the integral directly from MD simulation of water, I have to do the following modifications: for each frame k from the simulation, find all unique combination of pairs of molecules within distance R and sum up their contributions to the Fourier transform. R has to be chosen since the size of the simulation box is finite. Hence an estimate of $S(\vec{q})$ from one simulation frame is:

$$S(\vec{q}) \approx \frac{1}{N} \sum_{i,j=1}^N e^{-i\vec{q}\cdot(\vec{r}_i - \vec{r}_j)} \Delta_{ij} \quad (2)$$

where $\Delta_{ij} = 1$ if $|\vec{r}_i - \vec{r}_j| \leq R$ and is 0 otherwise.

Since liquid water is isotropic, intuition tells us that the pointing $(\vec{r}_i - \vec{r}_j)$ shouldn't matter and only its length should. Debye's formula formalizes this and the above summation is equivalent to:

$$S(Q) \approx \frac{1}{N} \sum_{i,j=1}^N \frac{\sin(Qr_{ij})}{Qr_{ij}} \Delta_{ij} \quad (3)$$

where $r_{ij} = |\vec{r}_i - \vec{r}_j|$ and Q is the magnitude of \vec{q} .

Averaging over many independent simulation frames gives an estimate from the simulation of $S(Q)$. There is also a finite-size effect introduced by the simulation box. See the two Salcuse papers in the notes for details. The finite-size effect is implemented in the code.

I have done some checking to make sure that the explicit Fourier transform makes sense with my simulation data. So far I have checked that it produces a small imaginary part, and also seems to be only dependent on the magnitude of \vec{q} but not its pointing. Also, equations 2 and 3 give the same answer when I use them to compute $S(Q)$ from averaging over independent frames from the simulations. This makes me think that I have been doing the explicit Fourier transform correctly for the radial distribution.

2 Direct Calculation of