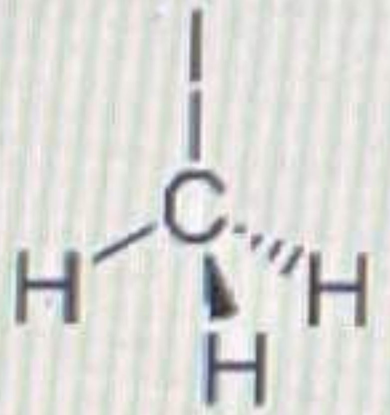
Question 3: (25 points) We have a solid iodomethane sample and would like to study its rotational and internal motions. The QENS signals are dominated by incoherent scattering of hydrogen atoms. The schematic picture of an iodomethane is shown in the figure too.



It is known that the normalized total intermediate scattering function can be approximated to be

$\tilde{I}(Q,t) = \tilde{I}_T(Q,t)\tilde{I}_R(Q,t)\tilde{I}_I(Q,t)$. Because we are interested in dynamics of solids, there is no center of mass translational motion. Hence, we can assume $\tilde{I}_T(Q,t) = 1$. Therefore, for our interest here, $\tilde{I}(Q,t) = \tilde{I}_R(Q,t)\tilde{I}_I(Q,t)$ where $\tilde{I}_R(Q,t)$ is for the rotational motion of the molecule, and $\tilde{I}_I(Q,t)$ is for the internal motions due to 3 site jumping of hydrogen atoms on a methyl group.

1) (**10 points**) The intermediate scattering function of the rotational motions can be approximated as

$$\tilde{I}_R(Q,t) = A_0(Q) + \sum_{l=1}^{\infty} A_l(Q)e^{-\frac{|t|}{\tau_l}}$$

where $A_0(Q) = j_0^2(QR^*)$, and $A_l(Q) = (2l+1)j_l^2(QR^*)$, R is the rotating radius, and $\frac{1}{\tau_l} = l(l+1)D_R$ with D_R to be the rotational diffusion coefficient.

Please find the expression of the dynamic structure factor, $\tilde{I}_R(Q,\omega)$, for the rotational motion. And what is the EISF for the rotational component. (Note that $\frac{1}{2\pi}\int e^{-|t|/\tau}e^{i\omega t}dt = \frac{1}{\pi}\frac{\tau}{(\omega\tau)^2+1}$.)

Please find the expression of the dynamic structure factor, $\tilde{I}_R(Q,\omega)$, for the rotational motion. And what is the EISF for the rotational component. (Note that $\frac{1}{2\pi}\int e^{-|t|/\tau}e^{i\omega t}dt = \frac{1}{\pi}\frac{\tau}{(\omega\tau)^2+1}$.)

2) (**5 points**) The three site jump motions due to hydrogen atoms on the methyl group can be expressed as $\tilde{I}_I(Q,t) = B_1(Q) + B_2(Q)e^{-\frac{3}{\tau}t}$, where $B_1(Q) = \frac{1}{3}(1 + 2j_0(QR\sqrt{3}))$ and $B_2(Q) = \frac{2}{3}(1 - j_0(QR\sqrt{3}))$, and τ is the average time a hydrogen atom stays at a site.

Please find what is the EISF if there is only the internal motion (jump diffusion).

3) (**10 points**) Please show the expression of the self-intermediate scattering function, $\tilde{I}(Q,t)$, by including both the rotational and internal dynamics. And also please find the expression for the EISF of this system (Elastic Incoherent Structure Factor). (Note that you can assume that $\tilde{I}_R(Q,t=0) = 1$ and $\tilde{I}_I(Q,t=0) = 1$.)

Question 4: (40 points) Neutron spin echo (NSE) is used to measure the diffusion of a samples that has two type of particles with uniform scattering length density. It is known that the scattering signal, $I(Q,t)$, is dominated by the coherent scattering. (It is ok if you do not know what is a NSE instrument yet. The question should have all the necessary details for you to have the answer.)

There are two types of spherical particles in solutions with radius of R_1 and R_2. The number density of these two types of particles are n_1 and n_2 respectively. The concentrations are low enough so that we do not need to worry about the inter-particle structure factor. And the scattering contrast for both particles with the solvent is $\Delta\rho$. The solvent viscosity is η. Note that all particles are subject to Brownian motions so that the Stokes-Einstein relation, $R = \frac{k_B T}{6\pi\eta D}$, where R is the radius, and D is the measured diffusion coefficient. The normalized form factor is $\tilde{P}(QR) = (\frac{3j_1(QR)}{QR})^2$ for a spherical particle with the radius R.

We hope to estimate the effective hydrodynamic radius measured by the NSE.

1)(**5 points**) Two types of particles are mixed together with the number density of n_1 and n_2. Please write the expression of the intermediate scattering function, $I(Q,t)$, of this mixture system. The final expression can only have the parameters given here: R_1 and R_2, n_1 and n_2, $\Delta\rho$, D_1 and D_2 where $D = \frac{k_B T}{6\pi\eta R}$.

2) **(15 points)** We use NSE to measure the apparent hydrodynamic radius. Because the NSE can measure $I(Q,t)$ at a wide Q range. The effective hydrodynamic radius depends on the Q value. In this question, we first focus on the low Q value where you can safely assume $\tilde{P}(QR) = 1$ where $\tilde{P}(QR) = \left(\frac{3j\ \ (QR\ \ )}{QR}\right)^2$ is the normalized form factor. By expanding $I(Q,t)$ obtained from 3.1 at the short time, t, as $I(Q,t) \approx I(Q,t=0)e^{-D_{eff}Q^2t} = I(Q,t=0)(1 - D_{eff}Q^2t)$, we can obtain the effect diffusion coefficient, from which, we can estimate the effective hydrodynamic radius, R_{eff}, using the given Stokes-Einstein relation. Please show that $D_{eff} = \frac{n_1 R_1{}^6 D_1 + n_2 R_2{}^6 D_2}{n_1 R_1{}^6 + n_2 R_2{}^6}$. And using the Stokes-Einstein relation, please find the results of R_{eff} (The final results for R_{eff} should only have four parameters: R_1 and R_2, n_1 and n_2,)

Here, you may need to use the following relationship: $e^{-DQ^2t} \approx 1 - DQ^2t$. **Note:** The final expression can only have the parameters given in the introduction of this question.

3) **(15 points)** When the Q value is very large, $\tilde{P}(QR) = \frac{9}{2}\frac{1}{Q^4R^4}$ based on the Porod's law scattering. We can still expand $I(Q,t)$ obtained from 3.1 at the short time, t, as $I(Q,t) \approx I(Q,t=0)(1 - D_{eff}Q^2t)$, at this Q range. Please derive the expression to calculate D_{eff} and R_{eff} at this Q range.

4) **(5 points)** If $R_1 = 2\,R_2$, the volume fraction of the two particles is the same, i.e., $n_1{R_1}^3 = n_2{R_2}^3$, please find the ratio of the effective radius between the value at low Q and high Q.