Problem Statement and formula constructor

The problem we want to solve is Spherical Average Exchange Hole:

$$\iint_{\Omega} \left(\vec{r}-\vec{P}\right)_x^i \left(\vec{r}-\vec{P}\right)_y^j \left(\vec{r}-\vec{P}\right)_z^k e^{-(\alpha+\beta)\left(\vec{s}-\left(\vec{P}-\vec{r}\right)\right)^2} d\theta d\varphi \tag{1.1}$$

Where the i, j, k are the random integers. And the integrate depends on $\bar{s}$.

First, we assume

$$\vec{Q}=\vec{r}-\vec{P}$$

And

$$r_Q=\vec{s}-\left(\vec{P}-\vec{r}\right)$$

So we have

$$\begin{aligned} x_Q &= \left(\vec{s}+\vec{Q}\right)_x \\ y_Q &= \left(\vec{s}+\vec{Q}\right)_y \\ z_Q &= \left(\vec{s}+\vec{Q}\right)_z \\ r_Q &= \vec{s}+\vec{Q} \end{aligned}$$

So the formula (1.1) can be rewritten as

$$\iint_{\Omega} x_Q^i y_Q^j z_Q^k e^{-(\alpha+\beta) r_Q^2} d\theta d\varphi \tag{1.2}$$

Let’s consider the formula inside the integrate

$$x_Q^i y_Q^j z_Q^k e^{-(\alpha+\beta) r_Q^2} \tag{1.3}$$

We suppose

$$\vec{Q}=\left(Q\sin\theta_0\cos\varphi_0 \quad Q\sin\theta_0\sin\varphi_0 \quad Q\cos\theta_0\right)^T$$

In polar coordinates.

Secondly, we fix z axis and rotate XOY plat.
So we have the coordinate convert:

$$\begin{pmatrix} x_Q^{'} \\ y_Q^{'} \\ z_Q^{'} \end{pmatrix} = \begin{pmatrix} \cos\varphi_0 & \sin\varphi_0 & 0 \\ -\sin\varphi_0 & \cos\varphi_0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x_Q \\ y_Q \\ z_Q \end{pmatrix} \tag{1.4}$$

Let

$$A_1 = \begin{pmatrix} \cos\varphi_0 & \sin\varphi_0 & 0 \\ -\sin\varphi_0 & \cos\varphi_0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Then we fix y axis and rotate the XOZ plat.

So we have the coordinate convert:

$$\begin{pmatrix} x_Q'' \\ y_Q'' \\ z_Q'' \end{pmatrix} = \begin{pmatrix} \cos\theta_0 & 0 & -\sin\theta_0 \\ 0 & 1 & 0 \\ \sin\theta_0 & 0 & \cos\theta_0 \end{pmatrix} \begin{pmatrix} x_Q' \\ y_Q' \\ z_Q' \end{pmatrix} \tag{1.5}$$

Let

$$A_2 = \begin{pmatrix} \cos\theta_0 & 0 & -\sin\theta_0 \\ 0 & 1 & 0 \\ \sin\theta_0 & 0 & \cos\theta_0 \end{pmatrix}$$

Combine (1.4) and (1.5), we have

$$\begin{pmatrix} x_Q'' \\ y_Q'' \\ z_Q'' \end{pmatrix} = A \begin{pmatrix} x_Q \\ y_Q \\ z_Q \end{pmatrix} = \begin{pmatrix} \cos\theta_0\cos\varphi_0 & \cos\theta_0\sin\varphi_0 & -\sin\theta_0 \\ -\sin\varphi_0 & \cos\varphi_0 & 0 \\ \sin\theta_0\cos\varphi_0 & \sin\theta_0\sin\varphi_0 & \cos\theta_0 \end{pmatrix} \begin{pmatrix} x_Q \\ y_Q \\ z_Q \end{pmatrix} \tag{1.6}$$

Where

$$A = A_2 A_1$$

We also get the inverse of formula (1.4)

$$\begin{pmatrix} x_Q \\ y_Q \\ z_Q \end{pmatrix} = A^{-1} \begin{pmatrix} x_Q'' \\ y_Q'' \\ z_Q'' \end{pmatrix} \tag{1.7}$$

Now go back to formula (1.3) we have

$$\begin{aligned} x_Q^i y_Q^j z_Q^k e^{-(\alpha+\beta) r_Q^2} &= x_Q^i y_Q^j z_Q^k e^{-(\alpha+\beta)\left(\vec{s}+\vec{Q}\right)^2} \\ &= x_Q^i y_Q^j z_Q^k e^{-(\alpha+\beta)\left(\vec{s}^2+\vec{Q}^2+2\vec{s}\cdot\vec{Q}\right)} \end{aligned} \tag{1.8}$$

Let

$$\begin{aligned} \gamma &= \alpha+\beta \\ s &= |\vec{s}| \\ Q &= |\vec{Q}| \\ g &= e^{-(\alpha+\beta)\left(\vec{s}^2+\vec{Q}^2\right)+2(\alpha+\beta)\cdot s\cdot Q} \end{aligned}$$

And plug formula (1.7) into the formula (1.8)

$$\begin{aligned} x_Q^i y_Q^j z_Q^k e^{-(\alpha+\beta)\left(\vec{s}^2+\vec{Q}^2+2\vec{s}\cdot\vec{Q}\right)} &= g \times x_Q^i y_Q^j z_Q^k e^{-2\gamma\vec{s}\cdot\vec{Q}} \\ &= g \times \left(A_{11}^{-1} x_Q'' + A_{12}^{-1} y_Q'' + A_{13}^{-1} z_Q''\right)^i \left(A_{21}^{-1} x_Q'' + A_{22}^{-1} y_Q'' + A_{23}^{-1} z_Q''\right)^j \\ &\quad \left(A_{31}^{-1} x_Q'' + A_{32}^{-1} y_Q'' + A_{33}^{-1} z_Q''\right)^k e^{-2\gamma\vec{s}\cdot\vec{Q}-2\gamma sQ} \end{aligned}$$

Let’s we consider a simple form:

$$\left(a_1x+B_1\right)^i\left(a_2x+B_2\right)^j\left(a_3x+B_3\right)^k=\sum_{t=0}^{i+j+k} f'\left(t,i,j,k\right)x^t \tag{1.9}$$

Where

$$f'\left(t,i,j,k\right)=\sum_{l=\max\{0,t-(j+k)\}}^{\min\{i,t\}}\ \sum_{m=\max\{0,t-l-k\}}^{\min\{t-l,j\}} a_1^l a_2^m a_3^{t-l-m}\binom{i}{l}\binom{j}{m}\binom{k}{t-l-m}B_1^{i-l}B_2^{j-m}B_3^{k+l+m-t}$$

Then we can use this regression formula to construct the whole syntax since $B_s=b_sy+C_s$

So finally, the formula (1.2) can be transformed to

$$\sum_x\sum_y\sum_z f\left(l,m,n\right)\iint_\Omega x^l l^m z^n e^{-2\gamma\vec{s}\cdot\vec{Q}-2\gamma sQ}d\theta d\varphi \tag{1.10}$$

And in polar coordinate, we set

$$x=s\sin\theta\cos\varphi$$
$$y=s\sin\theta\sin\varphi$$
$$z=s\cos\theta$$

Then the formula (1.10) become

$$\sum_x\sum_y\sum_z F\left(l,m,n\right)\iint_\Omega \sin^{l+m}\theta\cos^n\theta\sin^m\varphi\cos^l\varphi e^{-2\gamma sQ(\cos\theta+1)}d\theta d\varphi \tag{1.11}$$

Part 2: Now we solve the small integrate part in formula (1.11)

For any given number i, j, k, l, α, compute the Integral of the following function:

$$F\left(\theta,\varphi\right)=\int_0^{2\pi}\int_0^{\pi}\sin^i\theta\cos^j\theta\sin^k\varphi\cos^l\varphi\cdot e^{-\mu(\cos\theta+1)}d\theta d\varphi \tag{1.12}$$

First, the integral for angel θ and ϕ can be totally separated as

$$F\left(\theta,\varphi\right)=\int_0^{\pi}\sin^i\theta\cos^j\theta\cdot e^{-\mu(\cos\theta+1)}d\theta\cdot\int_0^{2\pi}\sin^k\varphi\cos^l\varphi d\varphi \tag{1.13}$$

Let

$$\operatorname{int}\theta\left(\theta\right)=\int_0^{\pi}\sin^i\theta\cos^j\theta\cdot e^{-\mu(\cos\theta+1)}d\theta$$

$$\operatorname{int}\varphi\left(\varphi\right)=\int_0^{2\pi}\sin^k\varphi\cos^l\varphi d\varphi$$

So

$$F\left(\theta,\varphi\right)=\operatorname{int}\theta\left(\theta\right)\cdot\operatorname{int}\varphi\left(\varphi\right)$$

i. For the intθ

$$\operatorname{int}\theta\left(\theta\right)=\int_0^{\pi}\sin^i\theta\cos^j\theta\cdot e^{-\mu(\cos\theta+1)}d\theta \tag{1.14}$$

There are two cases:

Case 1: If i is an even number. Hence $i = 2i'$

$$
\begin{aligned}
\operatorname{int}\theta(\theta) &= \int_0^\pi \sin^{2i'}\theta\cos^j\theta\cdot e^{-\mu(\cos\theta+1)}d\theta \\
&= \int_0^\pi \left(1-\cos^2\theta\right)^{i'}\cos^j\theta\cdot e^{-\mu(\cos\theta+1)}d\theta \qquad (1.15)\\
&= \sum_{s=0}^{i'}(-1)^s\binom{i'}{s}\int_0^\pi \cos^{j+2s}\theta\cdot e^{-\mu(\cos\theta+1)}d\theta
\end{aligned}
$$

It can be simplified as when $t = j + 2s$

$$\int_0^\pi \cos^t\theta\cdot e^{-\mu(\cos\theta+1)}d\theta \qquad (1.16)$$

Suppose

$$I(n,u) = \int_0^\pi \cos^n\theta\cdot e^{-\mu(\cos\theta+1)}d\theta$$

This one have a regression function

$$
\begin{aligned}
e^{-\mu}\int_0^\pi \cos^t\theta\cdot e^{-\mu\cos\theta}d\theta &= e^{-\mu}\int_0^\pi \cos^{t-1}\theta\cdot e^{-\mu\cos\theta}d\sin\theta \\
&= e^{-\mu}\cdot\left(\sin\theta\cos^{t-1}\theta\cdot e^{-\mu\cos\theta}\Big|_0^\pi - \int_0^\pi \sin\theta d\cos^{t-1}\theta\cdot e^{-\mu\cos\theta}\right) \\
&= e^{-\mu}\left(0-\int_0^\pi \sin\theta\cdot\left((t-1)\cos^{t-2}\theta(-\sin\theta)e^{-\mu\cos\theta}+\cos^{t-1}\theta e^{-\mu\cos\theta}\cdot\mu\sin\theta\right)d\theta\right) \\
&= e^{-\mu}\left(-\int_0^\pi (t-1)\left(-\sin^2\theta\right)\cdot\cos^{t-2}\theta e^{-\mu\cos\theta}+\mu\sin^2\theta\cos^{t-1}\theta e^{-\mu\cos\theta}d\theta\right) \\
&= e^{-\mu}\left(\int_0^\pi (t-1)\left(1-\cos^2\theta\right)\cos^{t-2}\theta e^{-\mu\cos\theta}-u\left(1-\cos^2\theta\right)\cos^{t-1}\theta e^{-\mu\cos\theta}d\theta\right) \\
&= e^{-\mu}(t-1)\int_0^\pi \cos^{t-2}\theta\cdot e^{-\mu\cos\theta}d\theta - e^{-\mu}(t-1)\int_0^\pi \cos^t\theta\cdot e^{-\mu\cos\theta}d\theta \\
&\quad -e^{-\mu}\mu\int_0^\pi \cos^{t-1}\theta\cdot e^{-\mu\cos\theta}d\theta + e^{-\mu}\mu\int_0^\pi \cos^{t+1}\theta\cdot e^{-\mu\cos\theta}d\theta
\end{aligned}
$$

That is

$$I(t,\mu) = (t-1)I(t-2,\mu)-(t-1)I(t,\mu)-\mu I(t-1,\mu)+\mu I(t+1,\mu)$$

So the regression function is

$$I(n,\mu)=\frac{1}{\mu}\left((n-1)I(n-1,\mu)+\mu I(n-2,\mu)-(n-2)I(n-3,\mu)\right) \qquad (1.17)$$

So this regression function will help us to generate the value of the function. However, we still need to know the first three items of $I(n,\mu)$

When $n=0$

$$I(0,\mu)=\int_0^{\pi} e^{-\mu(\cos\theta+1)}d\theta \qquad (1.18)$$

We do some transform here and use the expansions.

$$I(0,\mu)=\int_0^{\pi} e^{-\mu(\cos\theta+1)}d\theta$$

$$=\int_0^{\pi} e^{-2\mu\cos^2\frac{\theta}{2}}d\theta$$

Assume $\theta'=\theta/2$

$$I(0,\mu)=2\int_0^{\pi/2} e^{-2\mu\cos^2\theta'}d\theta' \qquad (1.19)$$

Let $T=\cos\theta'$ that is $\theta'=\arccos T$

$$I(0,\mu)=2\int_0^{1} e^{-2\mu T^2}\frac{1}{\sqrt{1-T^2}}dT \qquad (1.20)$$

Now we use binomial series to expand $1/\sqrt{1-T^2}$

$$\frac{1}{\sqrt{1-T^2}}=\sum_{n=0}^{\infty}\frac{1\cdot 3\cdot\cdots\cdot(2n-1)}{2^n n!}T^{2n}$$

So

$$I(0,\mu)=2\sum_{n=0}^{\infty}\frac{1\cdot 3\cdot\cdots\cdot(2n-1)}{2^n n!}\int_0^{1} e^{-2\mu T^2}T^{2n}dT \qquad (1.21)$$

Let

When $n=1$

$$I(1,\mu)=\int_0^{\pi}\cos\theta\cdot e^{-\mu(\cos\theta+1)}d\theta \qquad (1.22)$$

When $n=2$

$$I(2,\mu)=\int_0^{\pi}\cos^2\theta\cdot e^{-\mu(\cos\theta+1)}d\theta \qquad (1.23)$$

Case 2: i is an odd number. Hence $i=2i''+1$

$$\begin{aligned}
\operatorname{int}\theta(\theta) &= \int_0^\pi \sin^{2i''+1}\theta\cos^j\theta\cdot e^{-\mu(\cos\theta+1)}d\theta \\
&= e^{-\mu}\int_0^\pi \left(1-\cos^2\theta\right)^{i''}\cos^j\theta\cdot e^{-\mu\cos\theta}d\left(-\cos\theta\right) \\
&= \sum_{s=0}^{i''}(-1)^{s+1}\cdot\binom{i''}{s}\cdot e^{-\mu}\int_0^\pi \cos^{j+2s}\theta\cdot e^{-\mu\cos\theta}d\cos\theta
\end{aligned} \tag{1.24}$$

What we concern is

$$e^{-\mu}\int_0^\pi \cos^{j+2s}\theta\cdot e^{-\mu\cos\theta}d\cos\theta \tag{1.25}$$

Let $j' = j + 2s$

We have

$$e^{-\mu}\int_0^\pi \cos^{j'}\theta\cdot e^{-\mu\cos\theta}d\cos\theta \tag{1.26}$$

Let $x' = \cos\theta$, we can convert (1.17) to

$$\begin{aligned}
e^{-\mu}\int_1^{-1} x'^{j'}\cdot e^{-\mu x'}dx' &= e^{-\mu x'-\mu}\cdot\sum_{s=0}^{j'}(-1)^{j'-s}\frac{j'!}{s!(-\mu)^{j'-s+1}}x'^s\Bigg|_1^{-1} \\
&= e^{-\mu x'-\mu}\cdot\sum_{s=0}^{j'}\frac{j'!}{s!\mu^{j'-s+1}}x'^s\Bigg|_{-1}^{1}
\end{aligned} \tag{1.27}$$

https://en.wikipedia.org/wiki/List_of_integrals_of_exponential_functions
(from https://en.wikipedia.org/wiki/List_of_integrals_of_trigonometric_functions)

ii. For the intϕ

$$\operatorname{int}\varphi(\varphi) = \int_0^{2\pi}\sin^k\varphi\cos^l\varphi d\varphi \tag{1.28}$$

There are two cases:
Case 1: at least one of k and l is odd.
Suppose k is odd. Hence $k = 2k'+1$
So we have

$$\begin{aligned}
\sin^k\varphi = \sin^{2k'+1}\varphi &= \left(\sin^2\varphi\right)^{k'}\cdot\sin\varphi \\
&= \left(1-\cos^2\varphi\right)^{k'}\sin\varphi
\end{aligned} \tag{1.29}$$

Plug formula (1.11) to (1.10), we have

$$\begin{aligned}\operatorname{int}\varphi(\varphi) &= \int_0^{2\pi}\left(1-\cos^2\varphi\right)^{k'}\sin\varphi\cos^l\varphi d\varphi \\ &= \int_0^{2\pi}\left(1-\cos^2\varphi\right)^{k'}\cos^l\varphi d\left(-\cos\varphi\right)\end{aligned} \tag{1.30}$$

Let $\nu=\cos\varphi$

So we have

$$\operatorname{int}\varphi(\varphi) = -\int_0^{2\pi}\left(1-\nu^2\right)^{k'}\nu^l d\nu \tag{1.31}$$

Case 2: both of k and l are even. Hence $k=2k'', l=2l''$

We use the relationship in double angle translate:

$$\sin^2\varphi=\frac{1-\cos(2\varphi)}{2}$$
$$\cos^2\varphi=\frac{1+\cos(2\varphi)}{2}$$

So

$$\begin{aligned}\operatorname{int}\varphi(\varphi) &= \int_0^{2\pi}\sin^k\varphi\cos^l\varphi d\varphi \\ &= \int_0^{2\pi}\sin^{2k''}\varphi\cos^{2l''}\varphi d\varphi \\ &= \int_0^{2\pi}\left(\frac{1-\cos 2\varphi}{2}\right)^{k''}\left(\frac{1+\cos 2\varphi}{2}\right)^{l''}d\varphi \\ &= 2^{-(k''+l''+1)}\int_0^{2\pi}\left(1-\cos 2\varphi\right)^{k''}\left(1+\cos 2\varphi\right)^{l''}d2\varphi \\ &= 2^{-(k''+l''+1)}\int_0^{2\pi}\sum_{i=0}^{k''}\binom{k''}{i}\cos^i 2\varphi(-1)^i\cdot\sum_{j=0}^{l''}\binom{l''}{j}\cos^j 2\varphi d2\varphi \\ &= 2^{-(k''+l''+1)}\sum_{t=0}^{k''+l''}f\left(t,k'',l''\right)\cdot\int_0^{2\pi}\cos^t 2\varphi d2\varphi\end{aligned} \tag{1.32}$$

where

$$g\left(t,k'',l''\right)=\sum_{s=\max\{0,t-l''\}}^{\min\{k'',t\}}\binom{k''}{s}\binom{l''}{t-s}(-1)^s \tag{1.33}$$

Let $\varphi'=2\varphi$, then

$$\int_0^{2\pi}\cos^t 2\varphi d2\varphi=\int_0^{\pi}\cos^t\varphi' d\varphi' \tag{1.34}$$

For formula (1.21), there is a regression function:

$$\int \cos^n x dx = \frac{\cos^{n-1} x \sin x}{n} + \frac{n-1}{n} \int \cos^{n-2} x dx$$

(From https://en.wikipedia.org/wiki/List_of_integrals_of_trigonometric_functions)
(Also see http://mathworld.wolfram.com/CosineIntegral.html)