Multiple scattering in an infinite medium

Study of the multiple elastic scattering problem based on the diffusion equation. The small angle approximation is not needed in this approach.

$$\frac{\partial f}{\partial s} + \bar{u}\cdot\bar{\nabla} f = N\int\left[f(\bar{x},\bar{u}',s) - f(\bar{x},\bar{u},s)\right]\sigma(\bar{u}\cdot\bar{u}')\,d\bar{u}' \quad (1)$$

f is the probability of finding the particle moving along the direction $\bar{u}'$ after having travel a pathlength s, if the particle was initially at $\bar{X}$ moving along $\bar{u}$. N is the density of scatterers. $\sigma(\bar{u}\cdot\bar{u}')$ is the elastic scattering cross section differential in the scattering angle $(\bar{u}\cdot\bar{u}')$. Notice that we are using a different notation for the scattering angle.

Boundary conditions: $f(\bar{x},\bar{u},0) = \delta(\bar{x})\,\delta(\bar{u}-\hat{R})$, which corresponds to a particle moving from the origin and along the Z axis.

Let's expand the solution in spherical harmonics,

$$f = \sum_{lm} f_{lm}(\bar{x},s)\, Y_{lm}(\bar{u}).$$

substitute it in the diffusion equation (1) and apply ortonormalization

$$\sum_{lm}\frac{\partial f_{lm}}{\partial s}\int Y_{lm}(\bar{u})\,Y^{*}_{\lambda\mu}(\bar{u})\,d\bar{u} + \sum_{lm}\bar{\nabla} f_{lm}\cdot\int Y_{lm}(\bar{u})\,\bar{u}\,Y^{*}_{\lambda\mu}(\bar{u})\,d\bar{u}$$

$$= N\left[\sum_{lm} f_{lm}\iint Y_{lm}(\bar{u}')\,\sigma(\bar{u}\cdot\bar{u}')\,Y^{*}_{\lambda\mu}(\bar{u})\,d\bar{u}\,d\bar{u}' + \sum_{lm} f_{lm}\iint Y_{lm}(\bar{u})\,\sigma(\bar{u}\cdot\bar{u}')\,Y^{*}_{\lambda\mu}\,d\bar{u}\,d\bar{u}'\right]$$

THE LEFT HAND SIDE OF THIS EQUATION YIELDS

$$\frac{\partial f_{\lambda\mu}}{\partial s} + \sum_{lm} \bar{\nabla} f_{lm} \cdot Q_{\lambda\mu}^{lm}$$

INTERCHANGING INDEXES:

$$\frac{\partial f_{lm}}{\partial s} + \sum_{\lambda\mu} \bar{\nabla} f_{\lambda\mu} \cdot Q_{lm}^{\lambda\mu}$$

WHERE $Q_{lm}^{\lambda\mu} = \int Y_{lm}^{*}\, \bar{u}\, Y_{\lambda\mu}\, d\bar{u}$

FOR SOLVING THE RIGHTHAND SIDE OF THE EQUATION, LET'S EXPAND THE CROSS SECTION IN LEGENDRE POLYNOMIALS

$$\sigma(\cos\psi) = \sum a_K P_K(\cos\psi); \quad \text{WHERE} \quad \cos\psi = \bar{u}\cdot\bar{u}'.$$

LET'S SOLVE THE FIRST TERM OF THE RHS OF THE DIFFUSION EQUATION:

$$N \sum_{lm} f_{lm} \int d\bar{u} \int d\bar{u}'\, Y_{lm}(\bar{u}')\, Y_{\lambda\mu}^{*}(\bar{u}) \sum_{K} a_K P_K(\cos\psi)$$

NOW, WE HAVE TO USE THE SPHERICAL HARMONICS ADDITION THEOREM TO SUBSTITUTE THE LEGENDRE POLYNOMIALS

$$= N \sum_{lm} f_{lm} \int d\bar{u} \int d\bar{u}'\, Y_{lm}(\bar{u}')\, Y_{\lambda\mu}^{*}(\bar{u}) \sum_{K} a_K \left(\frac{4\pi}{2K+1}\right) \sum_{n=-K}^{K} Y_{Kn}(\bar{u})\, Y_{Kn}^{*}(\bar{u}')$$

$$= N \sum_{lm} f_{lm} \sum_{K} \frac{4\pi a_K}{(2K+1)} \sum_{n=-K}^{K} \left[\int Y_{lm}(\bar{u}')\, Y_{Kn}^{*}(\bar{u}')\, d\bar{u}' \right] \underbrace{\int Y_{\lambda\mu}^{*}(\bar{u})\, Y_{Kn}(\bar{u})\, d\bar{u}}_{\delta_{\lambda K}\, \delta_{\mu n}}$$

$$= N \sum_{lm} f_{lm} \left(\frac{4\pi a_\lambda}{2\lambda+1}\right) \underbrace{\int Y_{lm}(\bar{u}')\, Y_{\lambda\mu}^{*}(\bar{u}')\, d\bar{u}'}_{\delta_{l\lambda}\, \delta_{m\mu}}$$

$$= N f_{\lambda\mu} \frac{4\pi a_\lambda}{2\lambda+1} = N f_{\lambda\mu} \left(\frac{\overset{2}{\cancel{4\pi}}}{\cancel{2\lambda+1}}\right) \left(\frac{\cancel{2\lambda+1}}{\cancel{2}}\right) \int P_\lambda(\cos\psi)\, \text{sen}\,\psi\, d\psi = \boxed{2\pi N f_{\lambda\mu} \int P_\lambda(\cos\psi)\, \text{sen}\,\psi\, d\psi}$$

For the second term of the RHS of equation, we get

$$N \sum_{lm} f_{lm} \int d\bar{u}' \underbrace{\int d\bar{u}\, Y_{lm}(\bar{u}) Y^*_{\lambda\mu}(\bar{u})}_{\delta_{l\lambda}\delta_{m\mu}} \sigma(\bar{u}\cdot\bar{u}')$$

Notice that σ depends on the scattering angle $(\bar{u}\cdot\bar{u}')$, not on the incidence direction $(\bar{u})$. In addition, we may consider the particle moving along the z axis so $d\bar{u}' \to d\cos\psi\, d\varphi$

$$= N f_{\lambda\mu}\, 2\pi \int \sigma(\cos\psi) \operatorname{sen}\psi\, d\psi$$, considering cylindrica symmetry

$$= 2\pi N f_{\lambda\mu} \int \sigma(\cos\psi)\, d\cos\psi$$

Finally, changing the indexes back to lm, we obtain:

$$\frac{\partial f_{lm}}{\partial s} + \sum_{\lambda\mu} \bar{\nabla} f_{\lambda\mu} \cdot Q_{lm}^{\lambda\mu} = f_{lm} \underbrace{2\pi N \int \sigma(\cos\psi)\left[P_l(\cos\psi) - 1\right] \operatorname{sen}\psi\, d\psi}_{-K_l}$$

$$(2) \quad \boxed{\frac{\partial f_{lm}}{\partial s} + K_l f_{lm} = -\sum_{\lambda\mu} \bar{\nabla} f_{\lambda\mu} \cdot Q_{lm}^{\lambda\mu}}$$

$$\boxed{\begin{array}{l} Q_{lm}^{\lambda\mu} = \int Y^*_{lm}(\bar{u})\, \bar{u}\, Y_{\lambda\mu}(\bar{u})\, d\bar{u} \\ K_l = 2\pi N \int \sigma(\psi)\left[1 - P_l(\cos\psi)\right] \operatorname{sen}\psi\, d\psi \end{array}}$$

The latter is the formal solution for the transport equation.

Notice that the solution is determined by the elastic scattering cross section.

BOUNDARY CONDITIONS

AS SAID BEFORE, THE PARTICLE IS INITIALLY MOVING AWAY THE POINT AT $\bar{X}=0$ AND ALONG THE Z AXIS.

$$f(\bar{x},\bar{u},0) = \delta(\bar{x})\,\delta(\bar{u}-\hat{k})$$

$$\sum_{lm} f_{lm}(\bar{x},0)\,Y_{lm}(\bar{u}) = \delta(\bar{x})\,\delta(\bar{u}-\hat{k})$$

$$\sum_{lm} f_{lm}(\bar{x},0)\int Y_{lm}(\bar{u})\,Y^{*}_{\lambda\mu}(\bar{u})\,d\bar{u} = \delta(\bar{x})\int_{4\pi}\delta(\bar{u}-\hat{k})\,Y_{\lambda\mu}(\bar{u})\,du$$

$$f_{\lambda\mu}(\bar{x},0) = \delta(\bar{x})\,Y_{\lambda\mu}(\hat{k}) \quad ; \quad Y_{\lambda\mu}(\psi) = Y_{\lambda\mu}(0)$$

Accounting for the cylindrical symmetry AND CHANGING INDEXES

$$f_l(\bar{x},0) = \delta(\bar{x})\,Y_{l0}(0)$$

(3) $$\boxed{f_l(\bar{x},0) = \left(\frac{2l+1}{4\pi}\right)^{1/2}\delta(\bar{x})}$$

THE ANGULAR DISTRIBUTION.

Let's obtain the angular distribution $F(\bar{u},s)$, which quantifies the probability of finding the particle scattering an angle $\bar{u}$ after having traveled a pathlength s.

Let's integrate eq. 2 over the whole space

$$\int \frac{\partial f_{\ell m}}{\partial s} d\bar{x} + \int K_\ell f_{\ell m} d\bar{x} = -\int \sum_{\lambda\mu} \bar{\nabla} f_{\lambda\mu} \cdot Q_{\ell m}^{\lambda\mu} d\bar{x}$$

$$\frac{\partial}{\partial s} \int f_{\ell m} d\bar{x} + K_\ell \int f_{\ell m} d\bar{x} = -\sum_{\lambda\mu} \bar{\nabla}\left[\int f_{\lambda\mu} d\bar{x}\right] \cdot Q_{\ell m}^{\lambda\mu}$$

$Q_{\ell m}^{\lambda\mu}$ depends only on angles and the gradient of a constant is zero, so that

(4) $$\frac{\partial F_\ell}{\partial s} + K_\ell F_\ell = 0 \; ; \quad \text{where } F_\ell \equiv \int f_{\ell m}(\bar{x},s) d\bar{x}$$ and the index m has been dropped due to the cylindrical symmetry.

Integrating eq. (4), we obtain:

$$\frac{\partial F_\ell}{F_\ell} = -K_\ell \partial s \longrightarrow F_\ell(s) = F_\ell(0) e^{-\int_0^s K_\ell ds}$$

$$F_\ell(0) = \int f_\ell(\bar{x},0) d\bar{x}, \quad \text{(see eq. 3)}$$

$$= \int \delta(\bar{x}) \left(\frac{2\ell+1}{4\pi}\right)^{1/2} d\bar{x}$$

$$\boxed{F_\ell(0) = \left(\frac{2\ell+1}{4\pi}\right)^{1/2}}$$

(5) $$\boxed{F_\ell(s) = \left(\frac{2\ell+1}{4\pi}\right)^{1/2} e^{-\int_0^s K_\ell ds}}$$

Then, the angular distribution can be obtained integrating the solution of the transport equation (1) over all space:

$$F(\bar{u},s) = \int f(\bar{x},\bar{u},s)\,d\bar{x}$$

$$= \int \sum_{lm} f_{lm}(\bar{x},s)\,Y_{lm}(\bar{u})\,d\bar{x}$$

Having into account the cylindrical symmetry

$$F(\bar{u},s) = \sum_{l} Y_{l0}(\bar{u}) \underbrace{\int f_{l0}(\bar{x},s)\,d\bar{x}}_{F_l(s)}$$

$$F(\bar{u},s) = \sum_{l} \left(\frac{2l+1}{4\pi}\right)^{1/2} P_l(\cos\psi) \left(\frac{2l+1}{4\pi}\right)^{1/2} e^{-\int_0^s k_l\,ds}$$

$$\boxed{F(\bar{u},s) = \sum_{l} \underbrace{\left(\frac{2l+1}{4\pi}\right)^{1/2} P_l(\cos\psi)}_{Y_{l0}(\bar{u})} \underbrace{\left(\frac{2l+1}{4\pi}\right)^{1/2} e^{-\int_0^s k_l\,ds}}_{F_l(s)}}$$

Angular distribution

$$\boxed{F(\bar{u},s) = \sum_{l} \left(\frac{2l+1}{4\pi}\right) P_l(\cos\psi)\, e^{-\int_0^s k_l\,ds}}$$

k_l depends on s through the energy dependence of the elastic scattering cross section ($\sigma(\cos\psi)$).

Let's determine the mean scattering angle.

$$\langle\cos\psi\rangle = \int F(\bar{u},s)\cos\psi\,\sin\psi\,d\psi\,d\varphi = \int F(\bar{u},s)\,P_1(\cos\psi)\sin\psi\,d\psi$$

$$= \cancel{2\pi} \sum_{l} \cancel{\left(\frac{2l+1}{4\pi}\right)} e^{-\int_0^s k_l\,ds} \underbrace{\int P_l(\cos\psi)\,P_1(\cos\psi)\sin\psi\,d\psi}_{\frac{2}{2l+1}\delta_{l1}}$$

$$\boxed{\langle\cos\psi\rangle = e^{-\int k_1\,ds}}$$

AND it is EASY to PROVE that

$$\boxed{\langle P_\ell(\cos\psi)\rangle = e^{-\int k_\ell ds}}$$

Spatial distributions

The average longitudinal displacement is another quantity of interest in Monte Carlo simulations. Let's determine it within this formalism.

Defining $g_\ell(z,s) \equiv \iint f_{\ell m}(\bar{x},s)\,dx\,dy$, we obtain

$$\frac{\partial}{\partial s}\underbrace{\int f_{\ell m}\,dx\,dy}_{g_{\ell m}} + k_\ell \underbrace{\int f_{\ell m}\,dx\,dy}_{g_{\ell m}} = -\sum_{\lambda\mu} \frac{\partial g_{\lambda\mu}}{\partial s}\left(Q_{\ell m}^{\lambda\mu}\right)_z$$

with boundary conditions

$$g_{\ell m}(z,0) = \iint f_{\ell m}(\bar{x},0)\,dx\,dy = \left(\frac{2\ell+1}{4\pi}\right)^{1/2}\delta(z)\text{; see EQ 3.}$$

which means that there is no dependence on φ so that

$$g_{\ell m}(z,0) = g_{\ell 0}(z,0) = g_\ell(z,0)$$

According to Bethe, Handbuck der Physik (1933), Vol 24/1 p.551

$$\left(Q_{\ell 0}^{\lambda 0}\right)_z = \frac{\ell\,\delta_{\ell-1,\lambda}}{(4\ell^2-1)^{1/2}} + \frac{(\ell+1)\,\delta_{\ell+1,\lambda}}{[4(\ell+1)^2-1]^{1/2}}$$

$$\left(Q_{\ell 0}^{\lambda 0}\right)_z = \alpha_\ell\,\delta_{\ell-1,\lambda} + \alpha_{\ell+1}\,\delta_{\ell+1,\lambda}$$

$$\frac{\partial g_\ell}{\partial s} + k_\ell g_\ell = -\sum_{\lambda\mu}\frac{\partial g_\lambda}{\partial s}\left[\alpha_\ell\,\delta_{\ell-1,\lambda} + \alpha_{\ell+1}\,\delta_{\ell+1,\lambda}\right]$$

(6) $$\boxed{\frac{\partial g_\ell}{\partial s} + k_\ell g_\ell = -\frac{\partial}{\partial z}\left[\alpha_\ell\, g_{\ell-1} + \alpha_{\ell+1}\, g_{\ell+1}\right] = 0}$$

Let's define $H_{\ell n}$

$$H_{\ell n} \equiv \int_{-\infty}^{\infty} g_\ell(z,s)\, z^n\, dz$$

and multiply eq. (6) by z^n and integrate by parts

$$\int \frac{\partial g_\ell}{\partial s} z^n dz + k_\ell \int g_\ell z^n dz + \int \underbrace{\frac{\partial}{\partial z}\left[\alpha_\ell g_{\ell-1} + \alpha_{\ell+1} g_{\ell+1}\right]}_{du} \underbrace{z^n}_{v} dz = 0$$

$$\left(\frac{\partial}{\partial s} + k_\ell\right) H_{\ell n} + \underbrace{\left(\alpha_\ell g_{\ell-1} + \alpha_{\ell+1} g_{\ell+1}\right) z^n \Big|_{-\infty}^{\infty}}_{0} - n \int \left(\alpha_\ell g_{\ell-1} + \alpha_{\ell+1} g_{\ell+1}\right) z^{n-1} dz = 0$$

it should converge to 0 in ∞.

(7) $$\left(\frac{\partial}{\partial s} + k_\ell\right) H_{\ell n} - n\left[\alpha_\ell H_{\ell-1,n-1} + \alpha_{\ell+1} H_{\ell-1,n-1}\right] = 0$$

Eq 7 can be solved in ascending order of n.
Let's solve it firstly for $n=0$

$$\left(\frac{\partial}{\partial s} + k_\ell\right) H_{\ell 0} = 0$$

$$H_{\ell 0} = H_{\ell 0}(0)\, e^{-\int_0^s k_\ell\, ds} \equiv H_{\ell 0}(0)\, K_\ell$$

$$H_{\ell 0}(0) = \int g_\ell(z,0)\, dz = F_\ell(0) = \left(\frac{2\ell+1}{4\pi}\right)^{1/2} \quad \text{(see eq. 5)}$$

(8) $$\therefore \boxed{H_{\ell 0}(s) = \left(\frac{2\ell+1}{4\pi}\right)^{1/2} K_\ell}$$

Then for $n=1$

(9) $$\left(\frac{\partial}{\partial s} + k_\ell\right) H_{\ell 1} - \left[\alpha_\ell H_{\ell-1,0} + \alpha_{\ell+1} H_{\ell-1,0}\right] = 0$$

GENERAL SOLUTION TO EQ. 9.

$$y' + p(x)\,y = Q(x)$$

$$y(x) = e^{-\int p(x)\,dx} \cdot \int Q(x)\, e^{\int p\,dx}\, dx + C$$

IN THIS CASE $p(s) = K_\ell$ AND $Q(s) = \alpha_\ell H_{\ell-1,0} + \alpha_{\ell+1,} H_{\ell-1,0}$.

THEN, ACCOUNTING FOR EQ. 8; UP TO A CONSTANT

$$H_{\ell 1} = e^{-\int K_\ell ds} \int \left[\alpha_\ell \left(\frac{2(\ell-1)+1}{4\pi}\right)^{1/2} R_{\ell-1} + \alpha_{\ell+1} \left(\frac{2(\ell+1)+1}{4\pi}\right)^{1/2} R_{\ell+1}\right] \frac{1}{R_\ell(s')}\, ds$$

$$H_{\ell 1} = R_\ell(s) \int_0^s \left[\underbrace{\frac{\ell}{(4\ell^2-1)^{1/2}} \left(\frac{2\ell-1}{4\pi}\right)^{1/2}}_{a_\ell} R_{\ell-1} + \underbrace{\frac{(\ell+1)}{[4(\ell+1)^2-1]^{1/2}} \left(\frac{2\ell+3}{4\pi}\right)^{1/2}}_{b_\ell} R_{\ell+1}\right] \frac{ds'}{R_\ell(s')}$$

$$a_\ell = \frac{\ell}{(4\pi)^{1/2}} \left[\frac{\cancel{2\ell-1}}{(\cancel{2\ell-1})(2\ell+1)}\right]^{1/2} = \frac{\ell}{\sqrt{4\pi(2\ell+1)}}$$

$$b_\ell = \frac{\ell+1}{(4\pi)^{1/2}} \left[\frac{2\ell+3}{4\ell^2+8\ell+4-1}\right]^{1/2} = \frac{\ell+1}{(4\pi)^{1/2}} \left[\frac{\cancel{2\ell+3}}{(2\ell+1)(\cancel{2\ell+3})}\right]^{1/2} = \frac{\ell+1}{\sqrt{4\pi(2\ell+1)}}$$

$\therefore$

(10) $$H_{\ell 1} = \frac{R_\ell(s)}{[4\pi(2\ell+1)]^{1/2}} \int_0^s \frac{[\ell R_{\ell-1} + (\ell+1) R_{\ell+1}]}{R_\ell}\, ds' + C$$

$H_{\ell 1}(0) = C = 0$ BECAUSE THE INITIAL POSITION OF THE PARTICLE IS $z=0$.

PLEASE, NOTICE THAT THERE IS A TYPO IN EQ. 26 OF LEWIS' PAPER. IN ADDITION, EQ. 10 AGREES WITH THAT SHOW IN OUR text BOOK (SEE PAGE 101 OF BICLAJEW'S BOOK).

(11) $$\boxed{H_{\ell 1} = \frac{R_\ell(s)}{\sqrt{4\pi(2\ell+1)}} \int_0^s \frac{\ell R_{\ell-1} + (\ell+1) R_{\ell+1}}{R_\ell}\, ds'}$$

THEN, WE CAN NOW DETERMINE $\langle z \rangle$

$$\langle z \rangle = \int f(\bar{x},\bar{u},s)\cdot z \, \sin\psi \, d\psi \, d\varphi \, d\bar{x}$$

$$= \int z \sum_{lm} f_{lm}(\bar{x},s) \, Y_{lm}(\bar{u}) \sin\psi \, d\psi \, d\varphi \, dx\,dy\,dz$$

m=0 DUE to CYLINDRICAL SYMMETRY.

$$= \sum_l (4\pi)^{1/2} \underbrace{\int Y_{l0}(\bar{u}) \, Y^*_{00}(\cos\psi) \sin\psi \, d\psi \, d\varphi}_{\delta_{l0}} \int z \, g_l(z,s) \, dz$$

$$= (4\pi)^{1/2} \int z \, g_0(z,s) \, ds \equiv (4\pi)^{1/2} H_{01}$$

$$\boxed{\langle z \rangle = (4\pi)^{1/2} H_{01}}$$

USING SOLUTION IN EQ. 11

$$\langle z \rangle = \cancel{(4\pi)^{1/2}} \frac{R_0(s)}{\cancel{(4\pi)^{1/2}}} \int_0^s \frac{R_1(s')\,ds'}{R_0(s)} \quad ; \quad R_0(s) = e^{-\int_0^s K_0(s')\,ds'} = 1.$$

$$\boxed{\langle z \rangle = \int_0^s R_1(s')\,ds'}$$

WHICH AGREES WITH EQ. 27 of LEWIS' PAPER.

WE CAN ALSO DETERMIN $\langle z \cos\psi \rangle$

$$\langle z\cos\psi \rangle = \int \sum_l f_{lm}(\bar{x},s) \, Y_{lm}(\bar{u}) \, z \underbrace{\cos\psi}_{\left(\frac{4\pi}{3}\right)^{1/2} Y^*_{10}} \sin\psi \, d\psi \, d\varphi \, dx\,dy\,dz$$

$$= \left(\frac{4\pi}{3}\right)^{1/2} \sum_l \underbrace{\int Y_{lm} Y^*_{10} \sin\psi \, d\psi \, d\varphi}_{\delta_{l1}} \int g_l(z,s) \, z \, dz$$

$$\boxed{\langle z\cos\psi \rangle = \left(\frac{4\pi}{3}\right)^{1/2} H_{11}(s)} = \cancel{\left(\frac{4\pi}{3}\right)^{1/2}} \cancel{\left(\frac{3}{4\pi}\right)^{1/2}} R_1(s) \int_0^s \frac{(R_0 + 2R_2)\,ds'}{R_1}$$

$$\boxed{\langle z\cos\psi \rangle = R_1(s) \int_0^s \frac{1 + 2R_2(s')}{R_1(s')} ds'}$$

$\rightarrow$ EQ. 28 IN LEWIS' PAPER