Project Goal VGF Code

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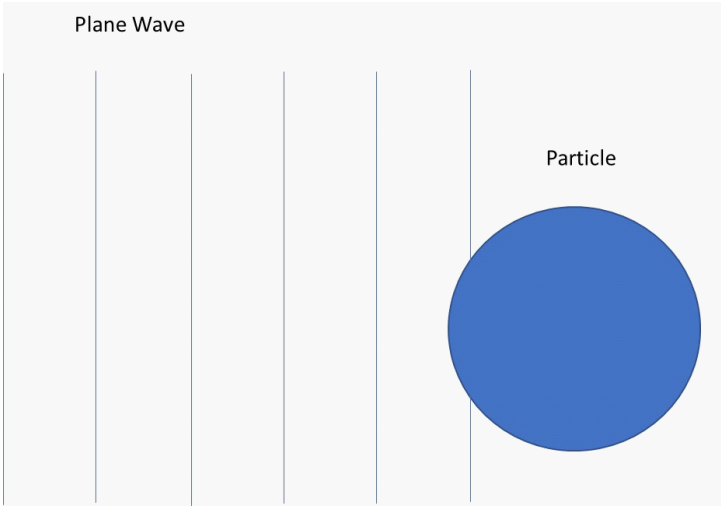
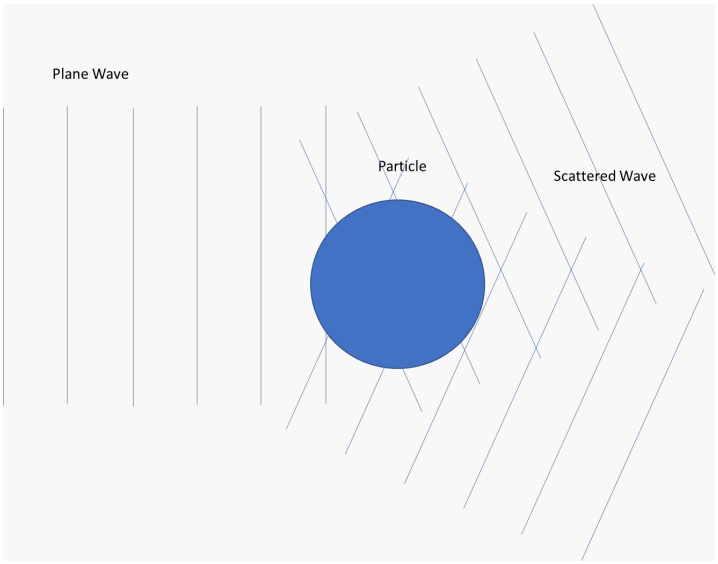
April 2, 2022

1 What we want to do

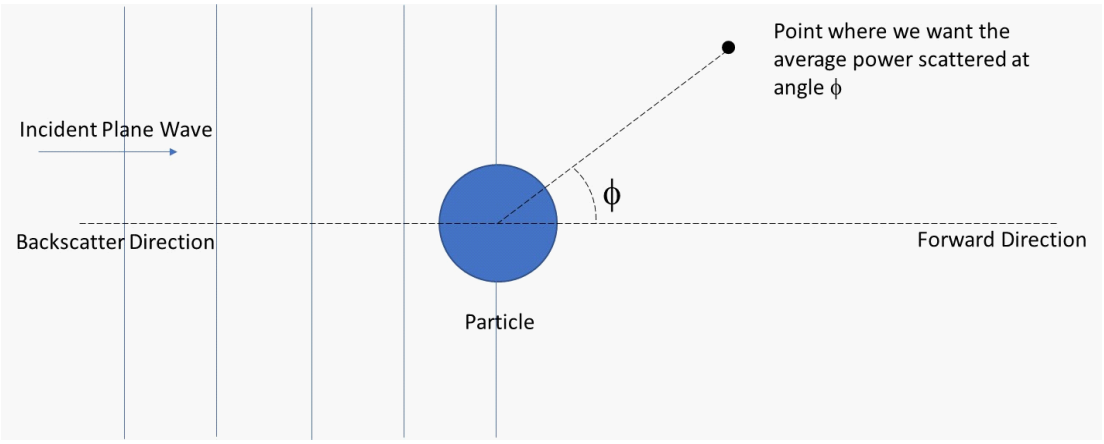
We want to calculate the average power scattered into a single direction when light hits a small particle. Let's assume a plane wave incident on a particle.



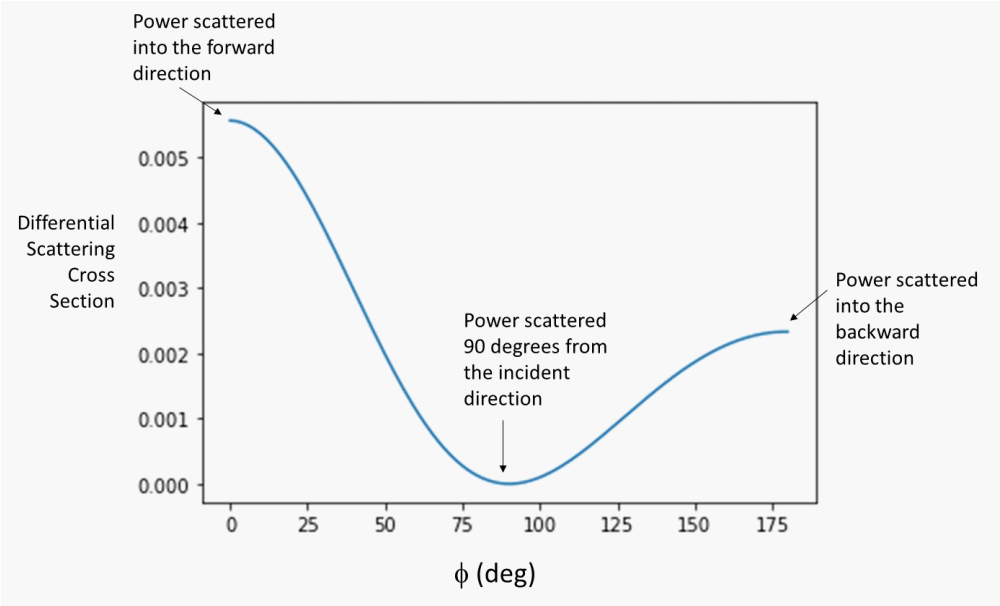
The light will scatter off of the particle in different directions.



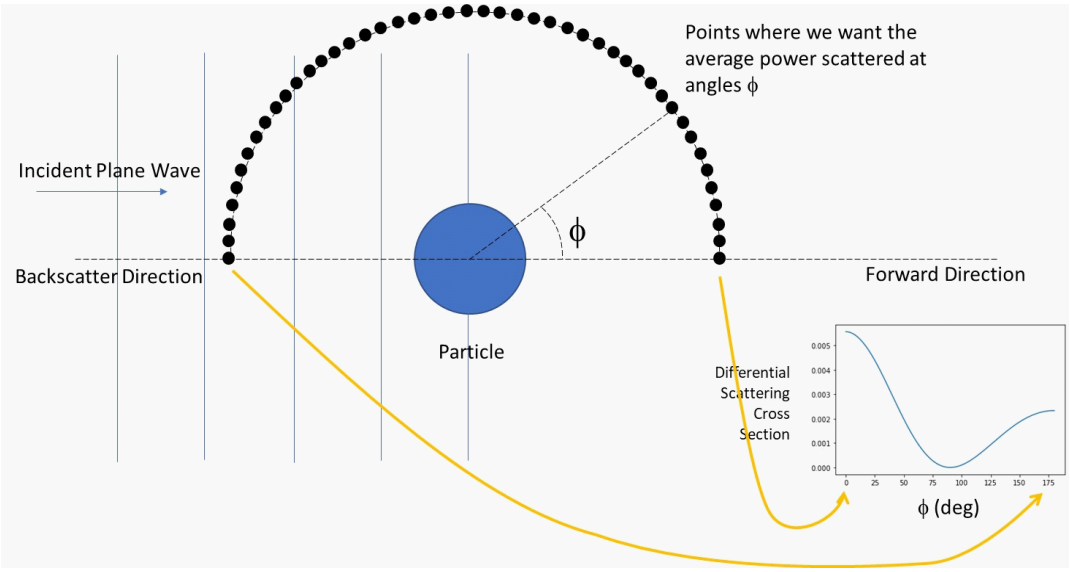
We want to get specific about this and to pick a measure of how strong the scattered field is that is sent off in a particular direction. Let's say we pick a plane that goes through the particle and has the incident wave perpendicular to the plane. We could pick a point on that plane and find the field or, because it is tradition, we could find the average power scattered into that direction.



And if we do this in a circle around the particle we get a good idea of how strong the field must be that is scattered from the particle. And we could graph this average power scattered into an angle.



where the value of the graph at $\phi = 0\,^\circ$ is the power that scatters in the same direction of the incident wave (the forward direction) and at $\phi = 180\,^\circ$ is the amount of power that scatters backward (back scatter).



In the example, there is a lot of forward scatter and a good amount of backscatter, but very little scatter at $\phi = 90\,^\circ$.

The power scattered into a specific direction is called the *differential scattering cross section.* This is what we will calculate.

To do the calculation we need to solve for the fields. Power will be proportional to the field squared. So we need the fields. The fields can be calculated using a Green's function approach.

$$\mathbf{E}(\mathbf{r})(1+\frac{4\pi}{3}\chi) = \mathbf{E}^e(\mathbf{r}) + \int d^3\mathbf{r}'\mathbf{G}\left(\mathbf{r},\mathbf{r}'\right)\cdot\chi(\mathbf{r}')\mathbf{E}(\mathbf{r}') \tag{1}$$

where the Green's function comes from Poisson's equation of electrostatics

$$\nabla^2 G\left(\mathbf{r}\right) = \frac{\rho\left(\mathbf{r}\right)}{\varepsilon_o}$$

This equation has solutions like

$$\nabla^2 G\left(\mathbf{r}\right) = \frac{1}{4\pi\varepsilon_o}\int \frac{\rho\left(\mathbf{r}'\right)}{|\mathbf{r}-\mathbf{r}'|}d\tau'$$

integrated over the volume of the charge distribution. The Green's function must solve the point source equation.

$$\nabla^2 G\left(\mathbf{r},\mathbf{r}'\right) = -4\pi\delta\left(\mathbf{r}-\mathbf{r}'\right)$$

And in general it has a form like

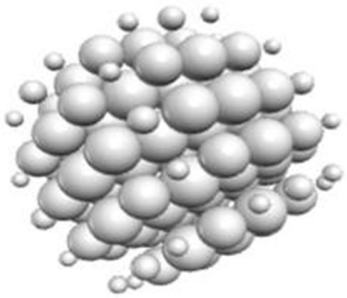
$$G\left(\mathbf{r},\mathbf{r}'\right) = \frac{1}{|\mathbf{r}-\mathbf{r}'|} + \Omega\left(\mathbf{r},\mathbf{r}'\right)$$

where V is a function that satisfies

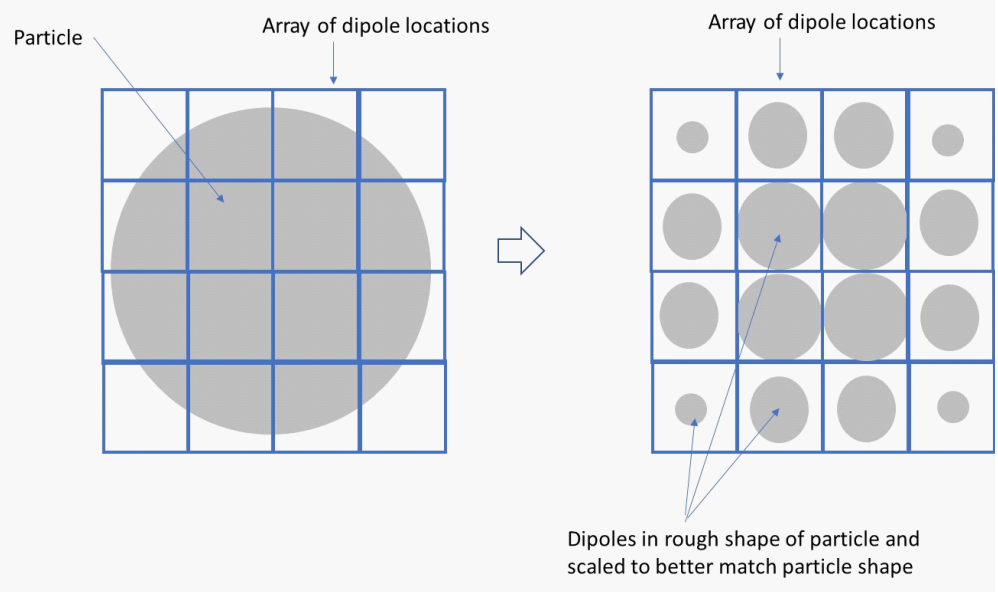
$$\nabla^2\Omega\left(\mathbf{r},\mathbf{r}'\right) = 0$$

Notice that we expect behavior kind of like $\frac{1}{|\mathbf{r}-\mathbf{r}'|}$ because electric fields have an inverse relationship to distance. But this is more complicated that just a field due to a point charge.

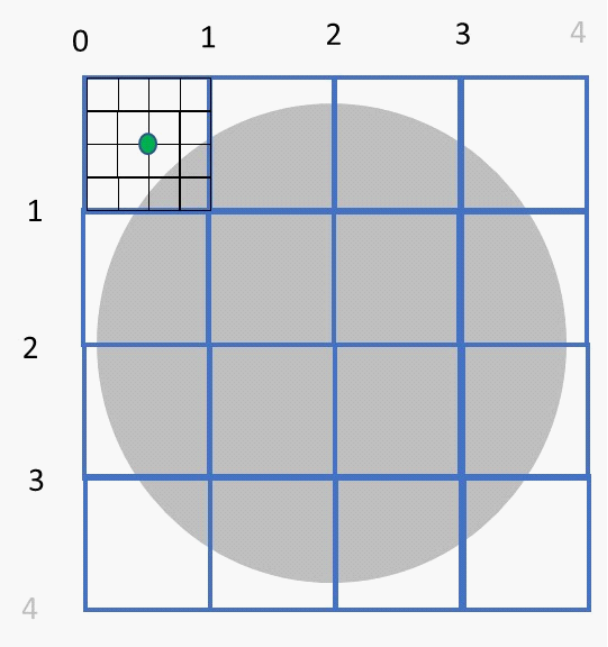
And equation (1) is hard to solve. To find a numeric solution we will make some approximations. First off we will split the particle up into pieces. Each piece we will approximate as a dipole scatterer because we know how to calculate scattering from dipoles. So a small spherical particle might look like this.



We need a method of defining the locations and the strength of each dipole scatterer. We will call this discretization the particle. Our method is to place the particle into a square matrix.



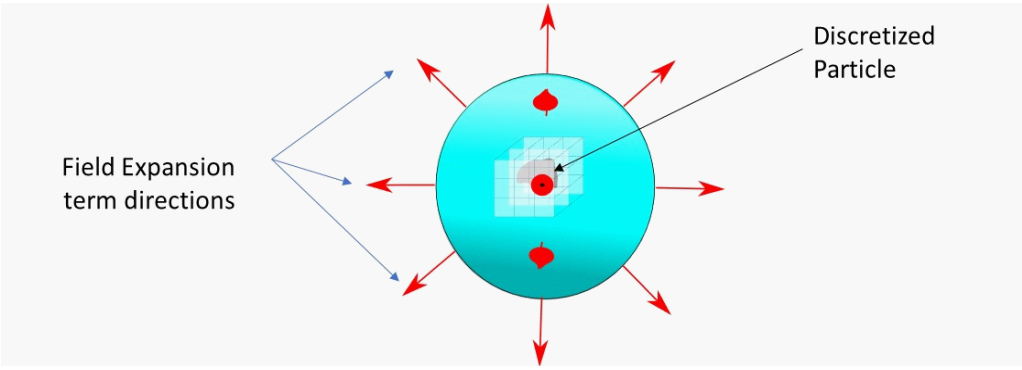
If a matrix cell has part of the particle in it, we will approximate it with a dipole scatterer. But we will weight each dipole by how much of the particle is inside the cell. So the cells in the corner of the matrix will be weighted less because there is only a little of the particle in the cell. To determine how much of the particle is in each cell, we divide up the cell into "fine structure" cells. And we count the number of fine structure cells that have part of the particle in them.



Once we have a digitized description of the particle we need to find the fields. But once again this it is hard to find the field in every direction. So we will calculate the field as a series expansion of plane wave fields. Each term will be a plane wave but each will have a different amplitude. And we will take a finite set of terms. These terms will can be in different directions. So we need to define at least a starting set of directions. Because plane waves are of the form.

$$\Psi_{\beta N} = Ae^{imk\hat{\mathbf{k}}_N \cdot \mathbf{r}_\beta}$$

where N tells us we have the Nth direction and where β tells us we are calculation the distance from the βth dipole, we will refer to the unit vectors in each of the expansion directions as k-vectors.



To calculate the fields from the dipole representation of the particle we need a discredited field equation. We will assume a field with complex time dependence.

$$\mathbf{E}\left(\mathbf{r},t\right)=\mathbf{E}(\mathbf{r})\exp(-i\omega t)+c.c. \tag{2}$$

and as usual never write the time dependence. We want to solve

$$\mathbf{E}(\mathbf{r})(1+\frac{4\pi}{3}\chi)=\mathbf{E}^{e}(\mathbf{r})+\int d^{3}\mathbf{r}'\mathbf{G}\left(\mathbf{r},\mathbf{r}'\right)\cdot\chi(\mathbf{r}')\mathbf{E}(\mathbf{r}') \tag{3}$$

We define the term

$$W\left(\mathbf{r}\right)=\frac{\chi(\mathbf{r})}{(1+\frac{4\pi}{3}\chi(\mathbf{r}))} \tag{4}$$

And for convenience define a new field that has the $W\left(\mathbf{r}\right)$ as part of it because the $W\left(\mathbf{r}\right)$ is tedious to write in all the equations.

$$\mathbf{F}(\mathbf{r})=\mathbf{E}(\mathbf{r})(1+\frac{4\pi}{3}\chi)$$

We will call this new field the F-field. So our field equation is now

$$\mathbf{F}(\mathbf{r})=\mathbf{E}^{e}(\mathbf{r})+\int d^{3}\mathbf{r}'\mathbf{G}\left(\mathbf{r},\mathbf{r}'\right)\cdot W\left(\mathbf{r}'\right)\mathbf{F}(\mathbf{r}') \tag{5}$$

And this is what we need to discretize. Since our particle is made of individual dipole scatterers, we can change the integral into a sum where we add up the field contribution for each dipole.

$$F_{\mu i}=E_{\mu i}^{in}+\sum_{\nu}G_{\mu i\nu j}W_{\nu}F_{\nu j} \tag{6}$$

where, for convenience, the cell dimension d_{μ}^{3} is included in the W term.

$$W_{\nu}=Wd_{\nu}^{3} \tag{7}$$

Symbolically, this may be written as

$$\mathbf{F}=\mathbf{E}^{in}+\mathbf{GWF} \tag{8}$$

If we knew the F-field and the incident field and the green's function we could solve this. But if we knew all of this we would already have the solution! But let's say we do know the fields, then we could write

$$0=\mathbf{F}-\mathbf{E}^{in}-\mathbf{GWF} \tag{9}$$

which seems obvious but unhelpful. But we want a numerical solution that is a series expansion. So we can guess that the F-field is a series expansion with plane waves as the basis of the expansion.

$$\tilde{F}_{\beta j}=\sum_{N=1}^{N_{k}}a_{Nj}\Psi_{\beta N} \tag{10}$$

But of course this isn't exactly right and we don't know the coefficients a_{Nj} so $\mathbf{F} - \mathbf{E}^{in} - \mathbf{GWF}$ won't be exactly zero. We could define an error term $\boldsymbol{\varepsilon}$ such that

$$\boldsymbol{\varepsilon} = \mathbf{F} - \mathbf{E}^{in} - \mathbf{GWF} \tag{11}$$

Writing components yields

$$\varepsilon_{\alpha i} = \sum_{\beta} \sum_{j} \left(1_{\alpha i \beta j} - G_{\alpha i \beta j} W_{\beta}\right) F_{\beta j} - E^{in}_{\alpha i} \tag{12}$$

Here the factor

$$F^{st}_{\alpha i} = -W_{\alpha} G_{\alpha i \alpha j} F_{\alpha j} \tag{13}$$

is the specially defined self term discussed below as the "self term." Note that

$$1_{\alpha i \beta j} = \delta_{\alpha \beta} \delta_{ij} \tag{14}$$

So we have made some progress. If we knew the coefficients a_{Nj} we could find out how bad our approximation is to the fields by calculating $\boldsymbol{\varepsilon}$. We want to make an attempt at this.

Now, because the equations are getting long, define the quantity

$$M_{\alpha i \beta j} = \left(1_{\alpha i \beta j} - W_{\beta} G_{\alpha i \beta j}\right) \tag{15}$$

where the α, i, β,and j are not summed over. Then

$$\varepsilon_{\alpha i} = \sum_{\beta} \sum_{j} \left(M_{\alpha i \beta j} F_{\beta j} - E^{o}_{\alpha i}\right) \tag{16}$$

which looks shorter.

But thinking of our notation for fields, the quantity $\varepsilon_{\alpha i}$ has complex components and is not a single value. It would be easier if we had a real number that told us how big our error in calculating the fields would be. So let's define a new function

$$\Phi = \sum_{\alpha} \sum_{i} \boldsymbol{\varepsilon}_{\alpha i} \boldsymbol{\varepsilon}^{*}_{\alpha i}$$

which would be real because of the conjugate multiply and would be a single number because of the sums. We want to minimize Φ.

$$\Phi = \sum_{\alpha} \sum_{i} \left(\sum_{\beta} \sum_{j} \left(M_{\alpha i \beta j} F_{\beta j} - E^{o}_{\alpha i}\right) \right) \left(\sum_{\gamma} \sum_{l} \left(M_{\alpha i \gamma l} F_{\gamma \lambda} - E^{o}_{\alpha i}\right) \right)^{*} \tag{17}$$

or

$$\Phi = \sum_{\alpha} \sum_{i} \boldsymbol{\varepsilon}_{\alpha i} \boldsymbol{\varepsilon}^{*}_{\alpha i} = \sum_{\alpha} \sum_{i} \sum_{\beta} \sum_{j} \sum_{\gamma} \sum_{l} \left(F_{\beta j} M^{T}_{\beta j \alpha i} M^{*}_{\alpha i \gamma l} F^{*}_{\gamma l} - E^{o*}_{\alpha i} M_{\alpha i \beta j} F_{\beta j} - E^{o}_{\alpha i} M^{*}_{\alpha i \beta j} F^{*}_{\beta j} + E^{o}_{\alpha i} E^{o*}_{\alpha i}\right) \tag{18}$$

Which is getting long again. Again for convenience two additional quantities are defined which will shorten the notation

$$K_{\gamma l\beta j} = M^{*T}_{\gamma l\alpha i} M_{\alpha i\beta j} \tag{19}$$

$$X^{*}_{\beta j} = E^{o*}_{\alpha i} M_{\alpha i\beta j} \tag{20}$$

Then equation (18) can be written compactly as

$$\Phi = \sum_{\alpha}\sum_{i}\sum_{\beta}\sum_{j}\sum_{\gamma}\sum_{l}\left(F^{*}_{\gamma l}K_{\gamma l\beta j}F_{\beta j} - \left[X^{*}_{\beta j}F_{\beta j} + X_{\beta j}F^{*}_{\beta j}\right] + E^{o}_{\alpha i}E^{o*}_{\alpha i}\right) \tag{21}$$

And now we can put in our guess for F.

$$\tilde{F}_{\beta j} = \sum_{N=1}^{N_k} a_{Nj}\Psi_{\beta N} \tag{22}$$

The function $\tilde{\mathbf{F}}$ is substituted for $\mathbf{F}$. The functions $\Psi_{\beta N}$ we will assume to be of the form

$$\Psi_{\beta N} = e^{imk\hat{\mathbf{k}}_N\cdot\mathbf{r}_\beta} \tag{23}$$

which depend on the $\hat{\mathbf{k}}_N$

Then equation (18) is approximately given by

$$\Phi = \sum_{\alpha}\sum_{i}\sum_{\beta}\sum_{j}\sum_{\gamma}\sum_{l}\sum_{N=1}^{N_k}\sum_{M=1}^{N_k}\left(\Psi^{*}_{\gamma M}a^{*}_{Ml}K_{\gamma l\beta j}a_{Nj}\Psi_{\beta N} - \left[X^{*}_{\beta j}\Psi_{\beta N}a_{Nj} + X_{\beta j}\Psi^{*}_{\beta N}a^{*}_{Nj}\right] + E^{o}_{\alpha i}E^{o*}_{\alpha i}\right) \tag{24}$$

Now the notation can again be simplified by defining two functions

$$H_{MlNj} = \sum_{\gamma}\sum_{\beta}\Psi^{*}_{\gamma M}K_{\gamma l\beta j}\Psi_{\beta N} \tag{25}$$

$$Y^{*}_{Nj} = \sum_{\beta}\Psi^{T}_{N\beta}X^{*}_{\beta j} \tag{26}$$

Then the final form of equation (18) is

$$\Phi = \sum_{\alpha}\sum_{i}\sum_{j}\sum_{l}\sum_{N=1}^{N_k}\sum_{M=1}^{N_k}a^{*}_{Ml}H_{MlNj}a_{Nj} - \left[Y^{*}_{Nj}a_{Nj} + Y_{Nj}a^{*}_{Nj}\right] + E^{o}_{\alpha i}E^{o*}_{\alpha i} \tag{27}$$

But we don't know the expansion coefficients a_{Nj} and a^{*}_{Ml}. We need to find these. We can use a variational technique. We can find a set of a_{Nj} and a^{*}_{Ml} that make Φ a minimum. An d we know how to find a minimum in an equation, we take a derivative and set it equal to zero.

Let's differentiate Φ with respect to a^{*}_{Li},

$$\frac{\partial\Phi}{\partial a^{*}_{Li}} = \sum_{\alpha}\sum_{i}\sum_{j}\sum_{l}\sum_{N=1}^{N_k}\sum_{M=1}^{N_k}a^{*}_{Ml}H_{MlNj}a_{Nj} - \left[Y^{*}_{Nj}a_{Nj} + Y_{Nj}a^{*}_{Nj}\right] + E^{o}_{\alpha i}E^{o*}_{\alpha i}$$

most terms drop out because a^*_{Li} is just one coefficient, so

$$\frac{\partial \Phi}{\partial a^*_{Li}} = \sum_{N=1}^{N_k} \sum_j \left(H_{LiNj} a_{Nj} - Y_{Li} \right) \tag{28}$$

and if we set this equal to zero we get

$$0 = \sum_{N=1}^{N_k} \sum_j \left(H_{LiNj} a_{Nj} - Y_{Li} \right) \tag{29}$$

$$\sum_{N=1}^{N_k} \sum_j H_{LiNj} a_{Nj} = Y_{Li} \tag{30}$$

can be written in matrix form as

$$\left(\mathbf{H} \right) \left(\mathbf{a} \right) = \left(\mathbf{Y} \right) \tag{31}$$

The solution for $(\mathbf{a})$ is given by

$$\left(\mathbf{a} \right) = \left(\mathbf{H} \right)^{-1} \left(\mathbf{Y} \right) \tag{32}$$

We can use a matrix solver to find a solution for the $(\mathbf{a})$ values. Then we can put them back ion

$$\tilde{F}_{\beta j} = \sum_{N=1}^{N_k} a_{Nj} e^{imk \hat{\mathbf{k}}_N \cdot \mathbf{r}_\beta} \tag{33}$$

to find the fields. The $\hat{\mathbf{k}}_N$ or "k-vectors" must be chosen to represent the internal wave well. A "goodness of choice" criterion for the number and direction of the $\hat{\mathbf{k}}_N$ vectors results from evaluating Φ explicitly. Observing the values of the a_{Nj} can determine which of the k-vectors are not contributing well. If the magnitude of an a_N is small, then the $\hat{\mathbf{k}}_N$ is not well placed or may not be needed.

For the sake of computation, a temporary variable is employed in the calculations that follow.

$$T_{\alpha i N j} = \sum_\beta \left(1_{\alpha i \beta j} - G_{\alpha i \beta j} W_\beta \right) \Psi_{\beta N} \tag{34}$$

Using $T_{\alpha i N j}$, H_{MlNj} and Y_{Nj} can be expressed as

$$\begin{aligned} H_{MlNj} &= \sum_\alpha \sum_i T^*_{\alpha i M l} T_{\alpha i N j} \\ Y_{Nj} &= \sum_\alpha \sum_i T^*_{\alpha i N j} E^o_{\alpha i} \end{aligned} \tag{35}$$

This is the form of the quantities used in the actual algorithms.

Then since we found the a_{Nj} with the matrix inversion we can calculate the

$$\tilde{F}_{\beta j} = \sum_{N=1}^{N_k} a_{Nj} e^{imk\hat{\mathbf{k}}_N \cdot \mathbf{r}_\beta} \tag{36}$$

and these are related to the electric field like this

$$\mathbf{F}(\mathbf{r}) = \mathbf{E}(\mathbf{r})(1 + \frac{4\pi}{3}\chi)$$

so

$$\frac{\mathbf{F}(\mathbf{r})}{(1 + \frac{4\pi}{3}\chi)} = \mathbf{E}(\mathbf{r})$$

and we have our electric field.

This is what the code is supposed to do.

2 Green's Functions

Let's return to the Green's function. The Green's function has the job of providing the field due to the scattering from one dipole to another.

$$\begin{aligned} F_i(\mathbf{r}_\mu) &= E_i^{in}(\mathbf{r}_\mu) + \sum_{\nu \neq \mu} d_\nu^3 G_{ij}(\mathbf{r}_{\mu\nu}) W F_j(\mathbf{r}'_\nu) + I_i(\mathbf{r}_\mu) \\ &= E_{\mu,i}^{in} + W \sum_{\nu \neq \mu} d_\nu^3 G_{\mu i \nu j} F_{\nu j} + I_{\mu i} \end{aligned} \tag{37}$$

Notice that the digitized form of the Green's function is summed over the number of dipoles. The index i is a specific vector component (say, the x-component) of the field scattered from a specific dipole, μ. The sum is over every dipole except dipole μ. So this equation gives the components of the field at a location due to the scattering from every dipole's own scattereing of the incident wave and the sattering from that dipole of the scattered waves from all the other dipoles. In the equation the sum does not include the particular dipole μ. So the sum gives us the field due to the dipole scattering the other dipoles scattered fields. The scattering of the incident field by dipole μ is separated out as a separate term $I_{\mu i}$. This scattering from dipole itself, is known as the "self term."

Recall that in the self therm $I_{\mu i}$, the Greek index tells the particular dipole, and the index i is the vector component. Of course, this only works well if d_μ^3 is small. Experience shows that $|m|\, kd < 1$ should be used, where m is the complex refractive index of the homogenous particle.

Let's now look at the form for the Green's function. The Green's function is discretized as

$$G_{\mu i \nu j} = \exp(ikR_{\mu\nu}) \left[\frac{k^2}{R_{\mu\nu}} \left(\delta_{ij} - \widehat{R_{\mu\nu i}} \widehat{R_{\mu\nu j}} \right) + \left(\frac{ik}{R_{\mu\nu}^2} - \frac{1}{R_{\mu\nu}^3} \right) \left(\delta_{ij} - 3\widehat{R_{\mu\nu i}} \widehat{R_{\mu\nu j}} \right) \right] \tag{38}$$

where $\mathbf{R}_{\mu\nu} = \mathbf{r}_\mu - \mathbf{r}_\nu$. This equation is very similar to that used by Goedecke and O'Brien.[1]

But a problem occurs when the summation index ν is equal to μ : Terms with $R_{\mu\mu}$ in the denominator would diverge (blow up to infinity). Thus in equation (37) these terms have been separated. Because such a term results from the action of the cell field on itself, it is known as the self-term. This is not as easy a term is it might apear. We can bordrow from Goodeke et. al[1] and others. The self-term results from letting $\mathbf{r} = \mathbf{r}_\mu$, and $\mathbf{r}' = \mathbf{r}_\mu + \boldsymbol{\xi}$, in equation (5) , and taking $\chi(\mathbf{r}')\mathbf{F}_j(\mathbf{r}') = \chi(\mathbf{r}_\mu)\mathbf{F}_j(\mathbf{r}_\mu)$. One gets

$$I_{\mu,i} = \left[\int_\square d^3\xi G_{ij}(\boldsymbol{\xi})\right] WF_j(\mathbf{r}_\mu) \tag{39}$$

The $\square$ indicates that the integral is over the small dipole cell, of volume d_μ^3. The integral in brackets in equation (**??**) can be written as

$$\int_\square d^3\xi G_{ij}(\boldsymbol{\xi}) = \int_\square d^3\xi e^{ik\xi}\left[\frac{k^2}{\xi}\left(\delta_{ij} - \hat{\xi}_i\hat{\xi}_j\right) + \left(\frac{ik}{\xi^2} - \frac{1}{\xi^3}\right)\left(\delta_{ij} - 3\hat{\xi}_i\hat{\xi}_j\right)\right] \tag{40}$$

Employing the identity

$$\int_\square d\Omega_\xi \hat{\xi}_i\hat{\xi}_j = \delta_{ij}\frac{1}{3}\int_\square d\Omega_\xi \tag{41}$$

the last term vanishes due to symmetry of cubical cells. Also, the remaining terms can be combined to yield

$$\int_\square d^3\xi G_{ij}(\boldsymbol{\xi}) = \delta_{ij}\frac{2k^2}{3}\int_\square d^3\xi\frac{k^2e^{ik\xi}}{\xi} \tag{42}$$

A series expansion of the integrand on the right hand side yields

$$\frac{\exp(ikx)}{x} = \left[\frac{1}{x} + ik - \frac{1}{2}k^2x - \frac{1}{6}ik^3x^2 + \frac{1}{24}k^4x^3 + Ox^4\right] \tag{43}$$

which can be substituted into the previous expression to yield

$$\begin{aligned}\int_\square d^3\xi G_{ij}(\boldsymbol{\xi}) &= \delta_{ij}\frac{2k^2}{3}\int_\square d^3\xi\left(\frac{1}{\xi} + ik - \frac{1}{2}k^2\xi - \frac{1}{6}ik^3\xi^2 + \frac{1}{24}k^4\xi^3 + O\left(\xi^4\right)\right)\\ &\equiv \delta_{ij}\frac{4\pi}{3}\Gamma\end{aligned} \tag{44}$$

where this equation defines Γ as

$$\Gamma = \left((ka)^2 + \frac{2}{3}i(ka)^3 - \frac{1}{4}(ka)^4 - \frac{1}{15}i(ka)^5 + O(ka)^6\right) \tag{45}$$

and the integral has been done by using an equivalent volume sphere with radius a_μ

$$a_\mu = d_\mu\left(\frac{3}{4\pi}\right)^{\frac{1}{3}} \tag{46}$$

thus

$$\Gamma_\mu = \left(\frac{3}{4\pi}\right)^{\frac{2}{3}} (kd_\mu)^2 + \left(\frac{i}{2\pi}\right)(kd_\mu)^3 - \frac{1}{4}\left(\frac{3}{4\pi}\right)^{\frac{4}{3}}(kd_\mu)^4 - \frac{1}{15}i\left(\frac{3}{4\pi}\right)^{\frac{5}{3}}(kd_\mu)^5 + O\left((kd_\mu)^6\right) \quad (47)$$

The expression for $I_{\mu i}$ can then be written as

$$I_{\mu i} = \delta_{ij}\frac{4\pi}{3}W\Gamma_\mu F_{\mu j} = \frac{4\pi}{3}W\Gamma_\mu F_{\mu i} \quad (48)$$

The first two terms in Γ_μ were used by Goedecke and O'Brien in their formulation of the DGF scattering code [1]. Draine and Goodman obtained a somewhat different expression for Γ_μ for placement of the dipole cells on a cubic lattice[2], i.e. the coefficients of the various powers of kd_μ are different than in equation(**??**). However, for ease in comparison with the DGF method, the form given by Goedecke and O'Brien is used here. The corrections of order $(kd_\mu)^4$and higher are insignificant; and even the term in $(kd_\mu)^2$ is not important if $kd_\mu \ll 1$. But, as shown by Goedecke and O'Brien, the lowest order imaginary term proportional to $(kd_\mu)^3$ is essential for agreement with the optical theorem, and this term is the same in the Draine and Goodman expression.

Putting this approximation for the Green's function into our equation for the F-field (Equation 6) gives us the mathematical representation used in the VGF code.

References

[1] G. H. Goedecke and S. G. O'Brien, "Scattering by irregular inhomogeneous particles via the digitized green's function algorithm," *Appl. Opt.*, vol. 27, no. 12, pp. 2431–2438, 15 June 1988.

[2] B. T. Draine and J. Goodman, "Beyond Clausius-Mossotti: Wave propagation on a polarizable point lattice and the discrete dipole approximation," *Astrophys. J.*, vol. 405, pp. 685–697, March 1993.