Scattering of Radiation with Polarization.

1. Stokes Parameters

The four parameters {I, Q, U, V} give a complete description of the polarized light relative to some reference axis. The degree of polarization is just $p = \sqrt{Q^2 + U^2 + V^2}/I$. The total intensity I is always positive, but Q, U and V may have negative values, as long as $[Q^2 + U^2 + V^2] \leq I^2$. The parameter V represents the circular polarization - its sign denotes right- or left-circular polarization. Q and U represent the amount $(Q^2 + U^2)$ and direction $(\tan 2\chi = U/Q)$ of the linear polarization. We assume we are looking along the direction of propagation, and the angle χ is measured counter-clockwise from the reference axis. Then if the light is 100% linearly polarized at 0^o (i.e., along the reference axis) the Stokes parameters are $\{1, 1, 0, 0\}$. If the plane of polarization is at an angle of 45^o, the parameters will be $\{1, 0, 1, 0\}$; at 90^o, $\{1, -1, 0, 0\}$; and at 135^o, $\{1, 0, -1, 0\}$. In fact the Q and U components of a 100% linearly polarized beam, which makes an angle χ with the reference axis (measured counter-clockwise looking along the direction of propagation) are given by $Q = \cos 2\chi$ and $U = \sin 2\chi$ (See Fig. 1).

Further, we can always represent any beam as the sum of an unpolarized component and a 100% polarized component:

$$\begin{bmatrix} I \\ Q \\ U \\ V \end{bmatrix} = \begin{bmatrix} (1-p)\ I \\ 0 \\ 0 \\ 0 \end{bmatrix} + \begin{bmatrix} p\ I \\ Q \\ U \\ V \end{bmatrix} \tag{1}$$

Here, p is the degree of polarization as defined above.

2. Transformation of the Stokes Parameters Under Rotation

If we rotate the direction of the reference axis, the total intensity I and circular polarization V are unchanged. We also see that $Q^2 + U^2$, and hence the *degree* of linear polarization, $\sqrt{Q^2 + U^2}/I$, is unchanged as well. The relative values of Q and U will change, however. We can write the transformation of the initial set of Stokes parameters $\{I, Q, U, V\}$ to a new set of parameters $\{I', Q', U', V'\}$ as a matrix multiplication. For a counter-clockwise rotation of the reference axis through an angle ϕ as viewed along the direction of propagation of the beam we have:

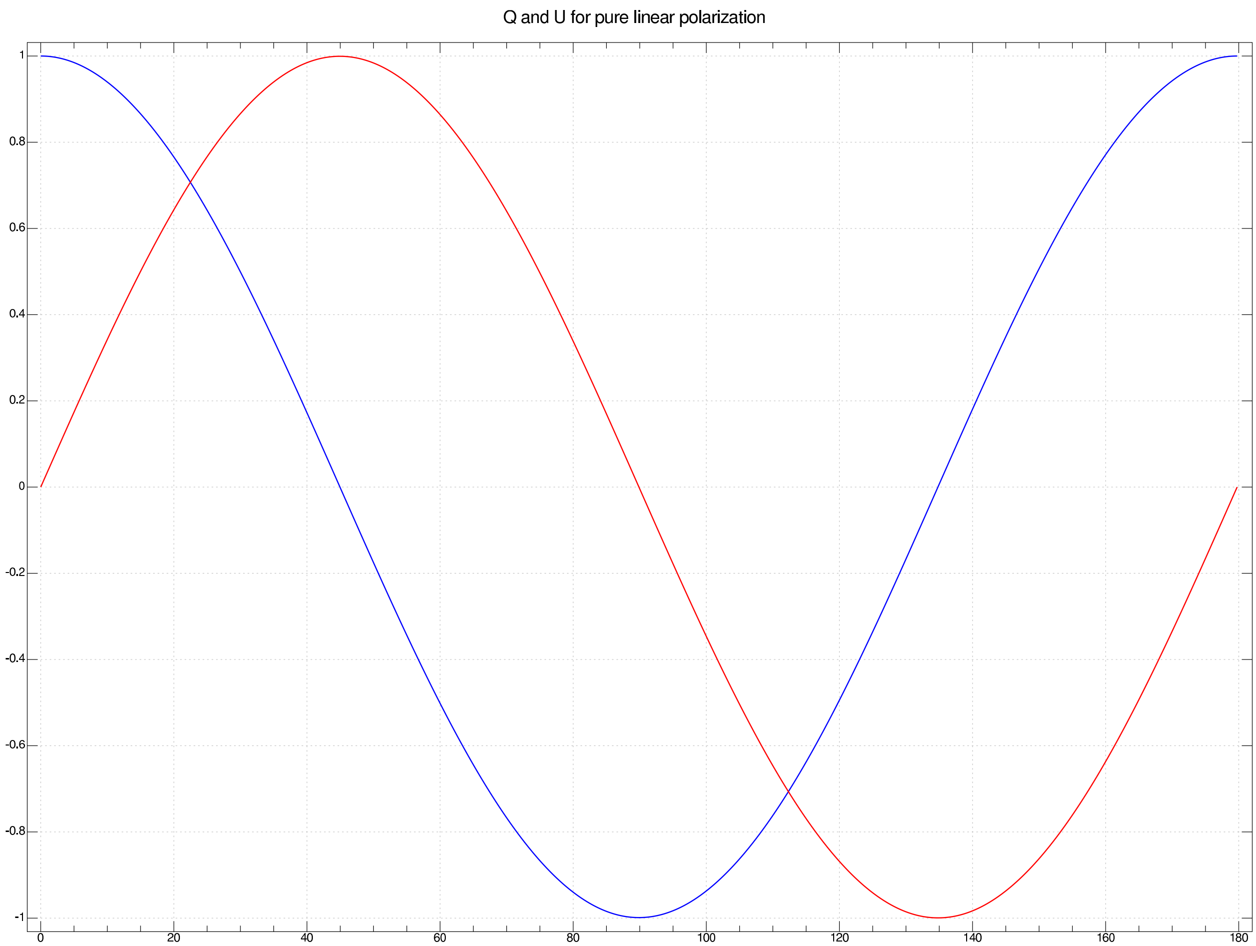

Fig. 1.— Variation of Q (blue) and U (red) with angle for pure linear polarization.

$$\begin{bmatrix} I' \\ Q' \\ U' \\ V' \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos 2\phi & \sin 2\phi & 0 \\ 0 & -\sin 2\phi & \cos 2\phi & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} I \\ Q \\ U \\ V \end{bmatrix} \tag{2}$$

Writing this out explicitly, $I' = I$,

$$Q' = Q \cos 2\phi + U \sin 2\phi \ , \tag{3}$$

$$U' = -Q \sin 2\phi + U \cos 2\phi \ , \tag{4}$$

and $V' = V$.

Suppose that $V = 0$. Then for Stokes parameters $\{I, Q, U, 0\}$, the angle between the reference axis and the plane of linear polarization, χ, is given by

$$\chi = \frac{1}{2} \arctan\left(\frac{U}{Q}\right) \ . \tag{5}$$

Note that *we must use a two-argument arctan function*: $U = Q = 1/\sqrt{2}$ corresponds to $\chi = 22.5^o$ while $U = Q = -1/\sqrt{2}$ must give $\chi = 112.5^o$, even though $(U/Q) = 1$ in both cases.

If we then rotate the reference axis counter-clockwise by χ, we see from eq. (3) & (4), using $\cos \arctan(x) = 1/\sqrt{1+x^2}$ and $\sin \arctan(x) = x/\sqrt{1+x^2}$, that $Q' = \sqrt{Q^2 + U^2}$ and $U' = 0$. Thus, with a rotation of the reference axis, it is possible to express any beam with partial linear polarization as a sum of unpolarized and completely polarized components:

$$\begin{bmatrix} I \\ Q \\ U \\ 0 \end{bmatrix} = (1-p)\ I \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} + p\ I \begin{bmatrix} 1 \\ 1 \\ 0 \\ 0 \end{bmatrix} \tag{6}$$

3. Rayleigh Scattering

In the case of Rayleigh scattering, where the Stokes parameters are referred to the scattering plane (i.e., a Stokes vector of {1, 1, 0, 0} corresponds to an incoming beam which is 100% polarized in the plane of scattering), the scattering matrix takes the form

$$\begin{bmatrix} I_s \\ Q_s \\ U_s \\ V_s \end{bmatrix} = \frac{3}{4} \begin{bmatrix} \cos^2\theta + 1 & \cos^2\theta - 1 & 0 & 0 \\ \cos^2\theta - 1 & \cos^2\theta + 1 & 0 & 0 \\ 0 & 0 & 2\cos\theta & 0 \\ 0 & 0 & 0 & 2\cos\theta \end{bmatrix} \begin{bmatrix} I_i \\ Q_i \\ U_i \\ V_i \end{bmatrix} \tag{7}$$

Here the constant (3/4) is such that the scattering is normalized for unpolarized radiation integrated over all angles. That is, the scattered intensity integrated over all directions equals the intensity of the incoming beam. We show this below.

3.1. Angle Averages of Rayleigh Scattered Radiation

Suppose we have a reference axis perpendicular to our beam, and relative to that axis the Stokes parameters are $\{I_i, Q_i, U_i, V_i\}$. The radiation may be scattered in any direction. The incoming and outgoing beams will define a plane: let it make an angle ϕ with reference axis. Within that plane, the outgoing beam makes an angle θ with the incoming beam ($\theta = \pi$ for backscatter). We want to integrate over the angles ϕ and θ. Since the Rayleigh scattering matrix is defined for Stokes parameters in the scattering plane, we must rotate the incoming parameters to that plane using eq (2). Thus the rotated (primed) parameters are

$$\begin{bmatrix} I_i' \\ Q_i' \\ U_i' \\ V_i' \end{bmatrix} = \begin{bmatrix} I_i \\ Q_i \cos 2\phi + U_i \sin 2\phi \\ -Q_i \sin 2\phi + U_i \cos 2\phi \\ V_i \end{bmatrix} \tag{8}$$

We then apply the scattering matrix (eq 7) to these parameters to obtain the parameters of the scattered beam:

$$\begin{bmatrix} I_s' \\ Q_s' \\ U_s' \\ V_s' \end{bmatrix} = \begin{bmatrix} \frac{3}{4}(\cos^2\theta + 1)I_i + \frac{3}{4}(\cos^2\theta - 1)(Q_i \cos 2\phi + U_i \sin 2\phi) \\ \frac{3}{4}(\cos^2\theta - 1)I_i + \frac{3}{4}(\cos^2\theta + 1)(Q_i \cos 2\phi + U_i \sin 2\phi) \\ \frac{3}{2}\cos\theta\ (-Q_i \sin 2\phi + U_i \cos 2\phi) \\ \frac{3}{2}\cos\theta\ V_i \end{bmatrix} \tag{9}$$

For a given orientation of the scattering plane, ϕ, we can integrate over all scattering angles θ. It is useful to make the variable change to $\mu = \cos\theta$. Then $d\mu = -\sin\theta\ d\theta$ and the desired integrals have the form

$$\frac{1}{4\pi}\int_0^{2\pi}\int_0^{\pi}\{I_s', Q_s', U_s', V_s'\}\ \sin\theta\ d\theta\ d\phi = \frac{1}{4\pi}\int_0^{2\pi} d\phi\ \int_{-1}^{1}\{I_s', Q_s', U_s', V_s'\}\ d\mu \quad . \tag{10}$$

The integrals over $\mu(= \cos\theta)$ have the values

$$\frac{1}{2}\int_{-1}^{1}(\mu^2+1)\ d\mu\ =\ \frac{4}{3}\ ,\quad \frac{1}{2}\int_{-1}^{1}(\mu^2-1)\ d\mu\ =\ -\frac{2}{3}\ ,\quad \frac{1}{2}\int_{-1}^{1}\mu\ d\mu\ =\ 0\ . \tag{11}$$

So the Stokes parameters integrated over μ in a given ϕ plane are

$$\begin{bmatrix} \overline{I'_s} \\ \overline{Q'_s} \\ \overline{U'_s} \\ \overline{V'_s} \end{bmatrix} = \frac{1}{2\pi} \begin{bmatrix} I_i - \frac{1}{2}(Q_i \cos 2\phi + U_i \sin 2\phi) \\ -\frac{1}{2} I_i + (Q_i \cos 2\phi + U_i \sin 2\phi) \\ 0 \\ 0 \end{bmatrix} \tag{12}$$

At this point, we see that for an unpolarized input beam, $\{I_i,\ 0,\ 0,\ 0\}$, the scattered radiation will be $(I_i/2\pi)\{1, -\frac{1}{2}, 0, 0\}$, independent of ϕ. The $\overline{Q'_s} = -1/2$ and $\overline{U'_s} = 0$ values indicate that the polarization is perpendicular to the plane of scattering.

Now since the reference axis varies with ϕ, we cannot simply integrate eqn (12) over that angle: we can only add Stokes parameters referred to the same axis. Thus we must first transform $\{\overline{I'_s}, \overline{Q'_s}, \overline{U'_s}, \overline{V'_s}\}$ back to the original axis by rotating by $-\phi$. Using eqn (2) and noting that $\sin(-2\phi) = -\sin(2\phi)$ and $\cos(-2\phi) = \cos(2\phi)$, the parameters referred to the original axis become

$$\begin{bmatrix} \overline{I_s} \\ \overline{Q_s} \\ \overline{U_s} \\ \overline{V_s} \end{bmatrix} = \frac{1}{2\pi} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos 2\phi & -\sin 2\phi & 0 \\ 0 & \sin 2\phi & \cos 2\phi & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} I_i - \frac{1}{2}(Q_i \cos 2\phi + U_i \sin 2\phi) \\ -\frac{1}{2} I_i + (Q_i \cos 2\phi + U_i \sin 2\phi) \\ 0 \\ 0 \end{bmatrix} \tag{13}$$

$$\begin{bmatrix} \overline{I_s} \\ \overline{Q_s} \\ \overline{U_s} \\ \overline{V_s} \end{bmatrix} = \frac{1}{2\pi} \begin{bmatrix} I_i - \frac{1}{2}(Q_i \cos 2\phi + U_i \sin 2\phi) \\ \cos 2\phi[-\frac{1}{2} I_i + (Q_i \cos 2\phi + U_i \sin 2\phi)] \\ \sin 2\phi[-\frac{1}{2} I_i + (Q_i \cos 2\phi + U_i \sin 2\phi)] \\ 0 \end{bmatrix} \tag{14}$$

In integrating this expression over the range $\phi = 0$ to $\phi = 2\pi$, the only non-vanishing integrals are

$$\int_0^{2\pi} d\phi = 2\pi \ , \quad \int_0^{2\pi} \cos^2 2\phi \ d\phi = \pi \ , \quad \text{and} \quad \int_0^{2\pi} \sin^2 2\phi \ d\phi = \pi \ . \tag{15}$$

Thus we finally obtain

$$\begin{bmatrix} \overline{\overline{I_s}} \\ \overline{\overline{Q_s}} \\ \overline{\overline{U_s}} \\ \overline{\overline{V_s}} \end{bmatrix} = \begin{bmatrix} I_i \\ \frac{1}{2} Q_i \\ \frac{1}{2} U_i \\ 0 \end{bmatrix} \tag{16}$$

We see that the normalization is preserved, as $\overline{\overline{I_s}} = I_i$. Why does the circular polarization vanish? Apparently, as much radiation is backscattered as forward scattered, and the reversal of the sign for backscattered radiation ($2\cos\theta < 0$ for $\theta > \pi/2$) results in complete cancellation. We also note that an unpolarized beam, {1, 0, 0, 0}, results in zero polarization for the integrated radiation: of course the radiation is strongly polarized perpendicular to the scattering plane, but the various polarization directions cancel out when integrated over all ϕ.

3.2. Finding the angular distributions for Monte Carlo calculations

If we have a normalized probability of scattering into some angle ϕ given by $f(\phi)$ over some range ϕ_l to ϕ_u, then consider the *cumulative distribution function* given by

$$F(\phi) \;=\; \int_{\phi_l}^{\phi\leq\phi_u} f(\phi')d\phi' \quad , \qquad \text{where} \qquad F(\phi_u) \;=\; 1 \quad . \tag{17}$$

The function F ranges over the interval $0 \leq F(\phi) \leq 1$.

Let r be a random number on the interval [0,1]. (Then $R = \phi_l + (\phi_u - \phi_l) * r$ will be uniformly distributed on the interval $[\phi_l, \phi_u]$.) Now if the function $F(\phi)$ can be inverted, then $\phi(r) = F^{-1}(r)$ will provide the probability of scattering into particular values of ϕ . Unfortunately, while $f(\phi)$ may be easy to invert, $F^{-1}(\phi)$ is usually not analytic.

3.3. Distribution of ϕ angles.

Let us examine the case of Rayleigh scattering. We first want find the distribution in the angle ϕ between the reference axis and the scattering plane. For unpolarized radiation, this must be just the uniform distribution $\phi = 2\pi\ r$. Since by eqn (6) we can express any incident beam as the sum of unpolarized and completely polarized components, it will suffice to consider the case $\{I_i, Q_i, U_i, V_i\} = \{1, 1, 0, v_i\}$. Then from eqn (14) we see that the intensity of the scattered radiation integrated over θ will be $\overline{I_s} = [1 - \frac{1}{2}\cos 2\phi]/2\pi$. This makes sense, as the $\overline{I_s}$ will be a minimum when $\phi = 0$, as this puts the plane of polarization in the scattering plane; $\overline{I_s}$ reaches a maximum for $\phi = \pi/2$, when the beam is polarized perpendicular to the scattering plane. Looking at the cumulative distribution function $F(\phi)$, we find

$$F(\phi) \;=\; \int_0^{\phi} \overline{I_s}(\phi')d\phi' \;=\; \frac{1}{2\pi}\int_0^{\phi}(1 - \frac{1}{2}\cos 2\phi')d\phi' \;=\; \frac{1}{2\pi}\left[\phi - \frac{1}{4}\sin 2\phi\right] \quad . \tag{18}$$

We see that $F(\phi)$ ranges over [0,1] as ϕ ranges from 0 to 2π, as it should. Now given uniformly random numbers r over the interval [0,1], to obtain the corresponding $\phi(r)$ we must solve

$$2\pi\ r \;=\; \phi \;-\; \frac{1}{4}\sin 2\phi \quad . \tag{19}$$

for ϕ. There is no analytic solution. For, if we define $E = 2\phi$ and $M = 4\pi\ r$, this equation becomes

$$M \;=\; E \;-\; \frac{1}{2}\,\sin E \quad , \tag{20}$$

which is just **Kepler's equation** for an eccentricity of $e = \frac{1}{2}$! In Fig. 2 we plot E as a function of M. The symmetry of the curve is more apparent when we plot G(M) = E(M)-M as a function of M, as in Fig. 3. $G(M) = 0$ for those values of E where $\sin E$ vanishes: $M = 0, \pi, 2\pi, 3\pi$ and 4π . We see from the symmetry of the curve that the solution of equation (20) for any $0 \leq M \leq 4\pi$ can be obtained from the solution on the interval $0 \leq M \leq \pi$. For if we define α and β as follows:

$0 \leq M \leq \pi$	$\alpha = 0$	$\beta = 1$
$\pi < M \leq 2\pi$	$\alpha = 2\pi$	$\beta = -1$
$2\pi < M \leq 3\pi$	$\alpha = -2\pi$	$\beta = 1$
$3\pi < M \leq 4\pi$	$\alpha = 4\pi$	$\beta = -1$

we can map M into $M' = \alpha + \beta \times M$, where $0 \leq M' < \pi$. Then, if G' is the solution for this M', we see that $E(M) = M + \beta \times G'$.

The simplest method of solution is to iterate $E_{n+1} = M + 0.5 * \sin E_n$. Tests show this seems always to converge, but often takes over 40 iterations to reach full machine accuracy. Simple Newton-Raphson also seems always to converge, and in only 6 iterations for full accuracy. The algorithm is

$$E_{n+1} \;=\; E_n \;+\; \frac{(M - E_n) + \frac{1}{2}\sin E_n}{1 - \frac{1}{2}\cos E_n} \quad , \quad \text{with} \qquad E_0 \;=\; M \quad . \tag{21}$$

Since we need only find G(M') over the interval $[0, \pi]$, we might try fitting this function with some approximation. We have tried a least-squares polynomial. Setting the constant term to zero forces the fit to have a zero at $M' = 0$, as it should. We also enforce a zero at $M' = \pi$. The coefficients for a 6th degree polynomial fit are:

$c_0 = 0, \quad c_1 = 1.092516365, \quad c_2 = -0.6952445333, \quad c_3 = 0.05051354154,$

$c_4 = 0.07996340757, \quad c_5 = -0.02929178498, \quad c_6 = 0.003160021201$

In Fig. 4 we show G(M') and this polynomial fit. The fit is close but hardly perfect: in Fig. 5 we plot the error ($Approx. - G(M)$). The error is less than ~0.005.

So to find a uniform sampling of scattering angles ϕ', we get random values $M = 4\pi\ r$ for $0 \leq r \leq 1$, then solve eqn (20) for E, and our sample is $\phi' = E/2$. Of course, since ϕ' is relative to the plane of polarization, we must then add the angle of the incoming polarization plane χ_i from eqn (5) to get the sampled angle relative to the reference plane: $\phi = \phi' + \chi_i$.

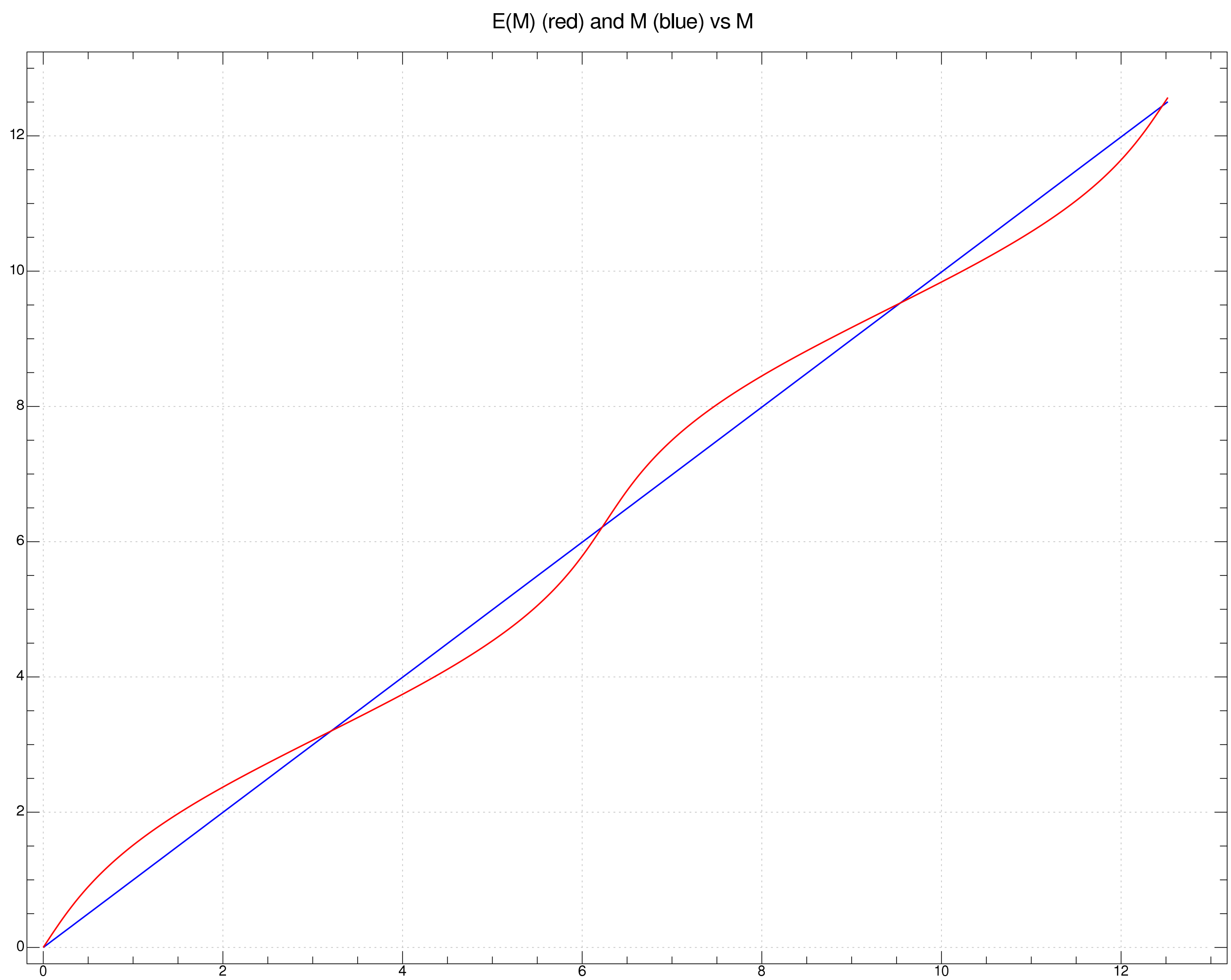

Fig. 2.— The the inverse of Kepler's equation (20).

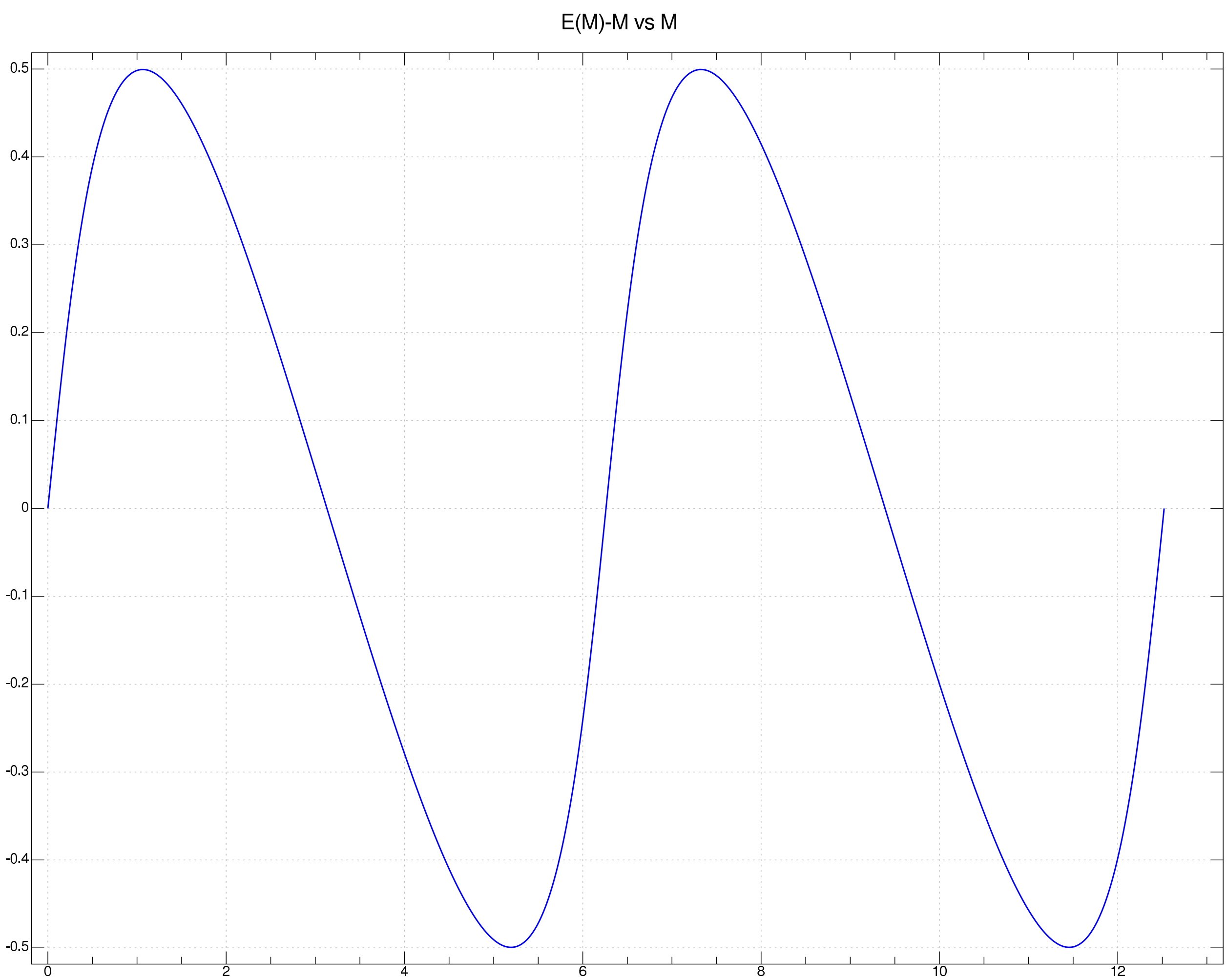

Fig. 3.— A plot of G(M) = E(M)-M in the interval [0,4π].

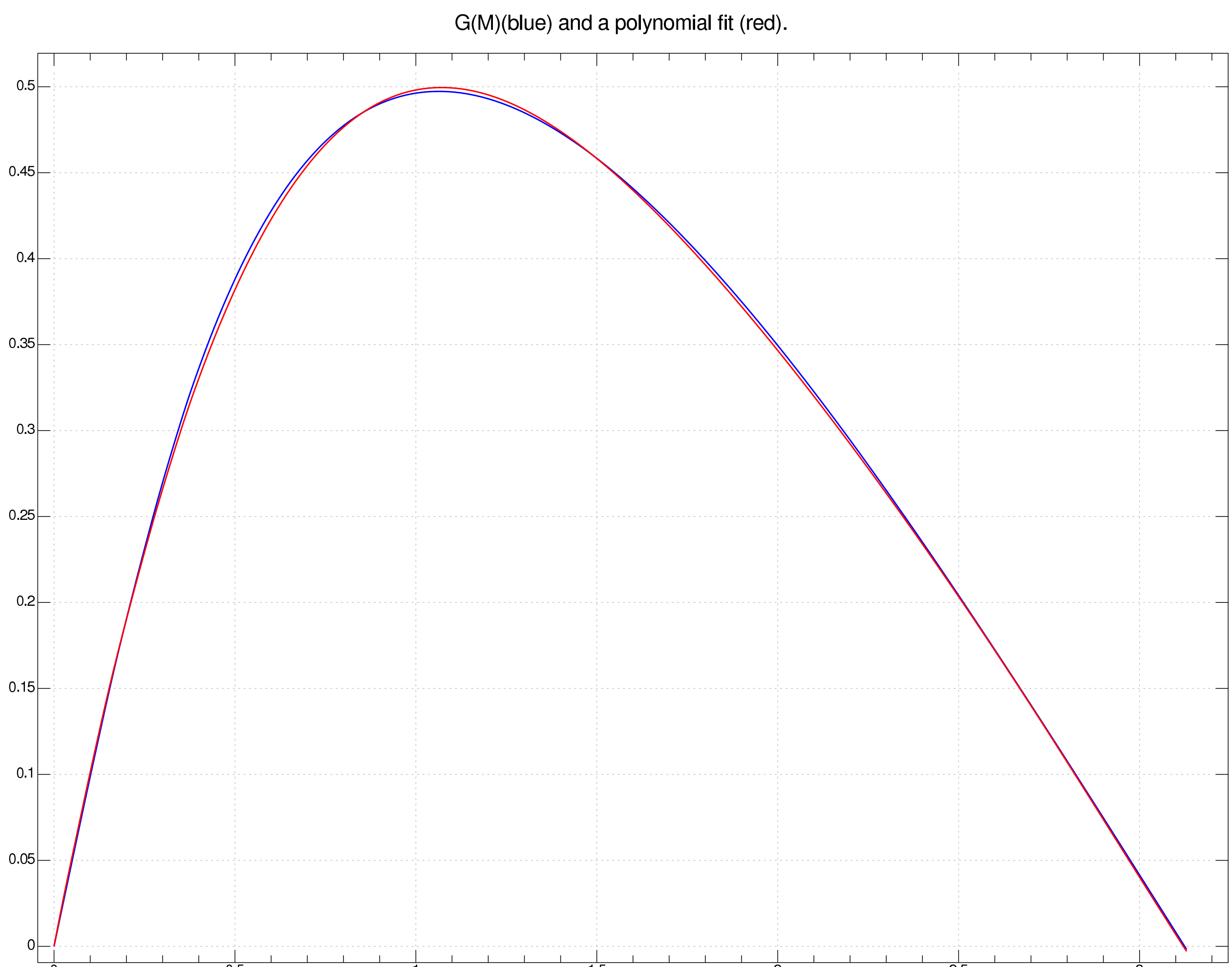

Fig. 4.— G(M)(=E(M)-M)(blue) and a polynomial fit (red) on the interval [0,π].

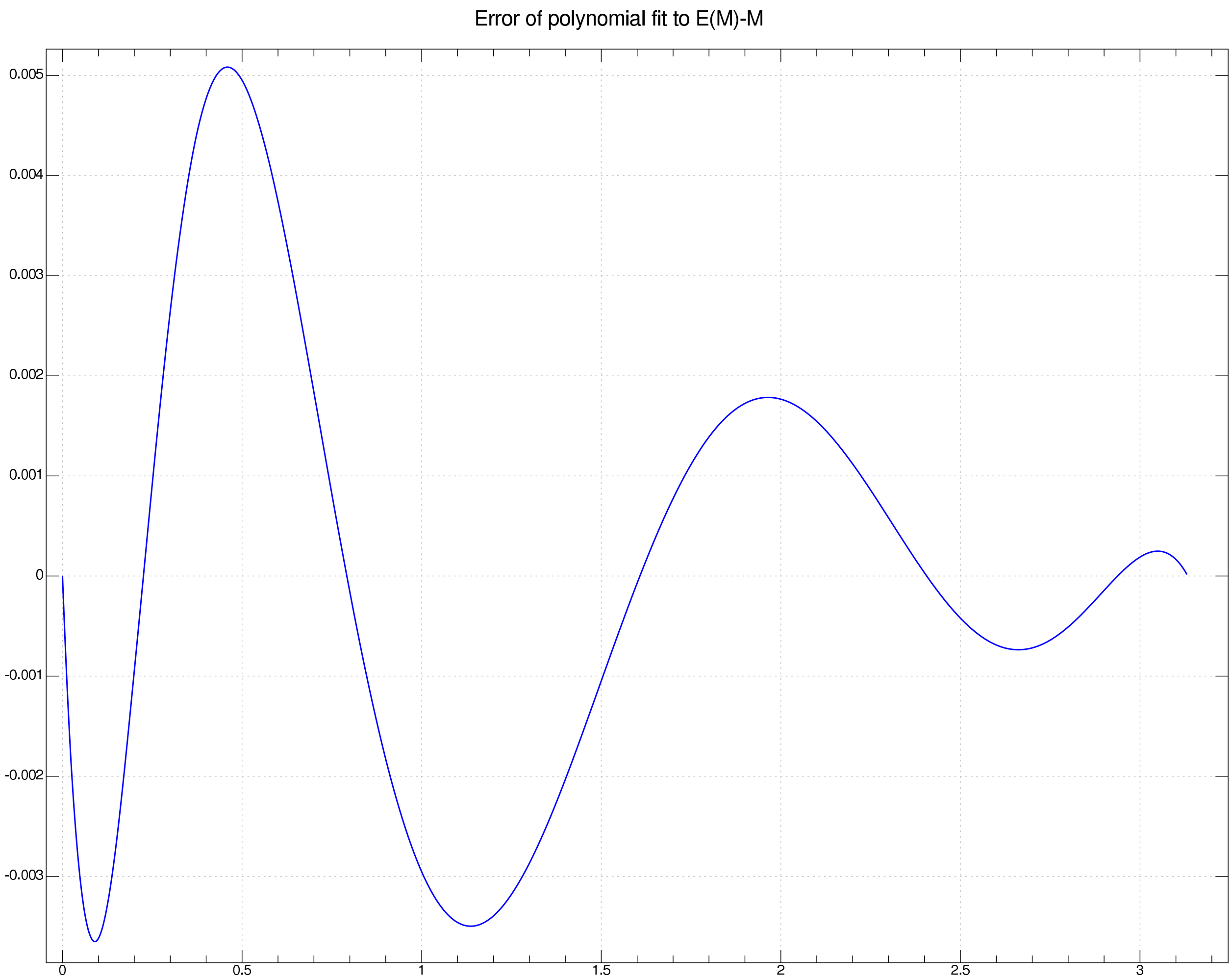

Fig. 5.— A plot of the error in the polynomial fit to G(M').

If the linear polarization is not complete, we can take the random number r, and if $0 \leq r < p$, apply the foregoing to $M = 4\pi(r/p)$, while if $p \leq r \leq 1$, we use a uniform distribution $\phi = 2\pi\ (1-r)/(1-p)$.

On the other hand, we may consider the case of partial polarization more directly. Assume we have rotated to the plane of polarization so that the Stokes parameters have the form $\{1, p, 0, v\}$. Then from eqn (14) we see that the intensity of the scattered radiation integrated over θ will be $\overline{I_s} = [1 - \frac{1}{2}p\ \cos 2\phi]/2\pi$. Then, as with equation (18), the cumulative distribution function $F(\phi)$ becomes

$$F(\phi) \ = \ \frac{1}{2\pi}\int_0^{\phi}(1 - \frac{1}{2}p\ \cos 2\phi')d\phi' \ = \ \frac{1}{2\pi}\left[\phi - \frac{p}{4}\sin 2\phi\right] \quad . \tag{22}$$

As a result, for an arbitrary degree of polarization p, equation (20) becomes

$$M \ = \ E \ - \ \frac{p}{2}\ \sin E \quad , \tag{23}$$

i.e., Kepler's equation for an eccentricity of $e = p/2$. The Newton-Raphson algorithm (eqn 21) continues to apply if we replace $\frac{1}{2}$ with $\frac{1}{2}p$.

3.4. Distribution of θ angles.

Let us suppose we have chosen a value of ϕ as outlined above. We now want to get a uniform sampling of θ, the scattering angle in the plane of scattering. From equations (9) we have $I'_s = \frac{3}{4}(\cos^2\theta + 1)I_i + \frac{3}{4}(\cos^2\theta - 1)(Q_i \cos 2\phi + U_i \sin 2\phi)$. With $\mu = \cos\theta$ and $\alpha = (Q_i/I_i)\cos 2\phi + (U_i/I_i)\sin 2\phi$, the cumulative distribution has the form

$$\frac{1}{2}\int_0^{\theta} I_s(\theta')\sin\theta' d\theta' \ = \ I_i\ \frac{3}{8}\int_{\mu}^{1}(\mu'^{\ 2} + 1) + \alpha(\mu'^{\ 2} - 1)\ d\mu' \ . \tag{24}$$

Integrating over [-1,1], we get the normalization factor

$$I_i\ \frac{3}{8}\int_{-1}^{1}(\mu^2 + 1) + \alpha(\mu^2 - 1)\ d\mu \ = \ \left(1 - \frac{\alpha}{2}\right)\ I_i \tag{25}$$

thus the normalized cumulative distribution is just

$$F(\mu) \ = \ \frac{1}{2-\alpha}\left\{1 - \frac{1}{4}\mu(3+\mu^2) - \alpha\left(\frac{1}{2} - \frac{1}{4}\mu(3-\mu^2)\right)\right\} \quad . \tag{26}$$

We want the distribution of $-1 \leq \mu \leq 1$ such that $F(\mu) = r$ where r is uniformly random over [0,1]. Upon expansion this leads to a cubic equation in μ :

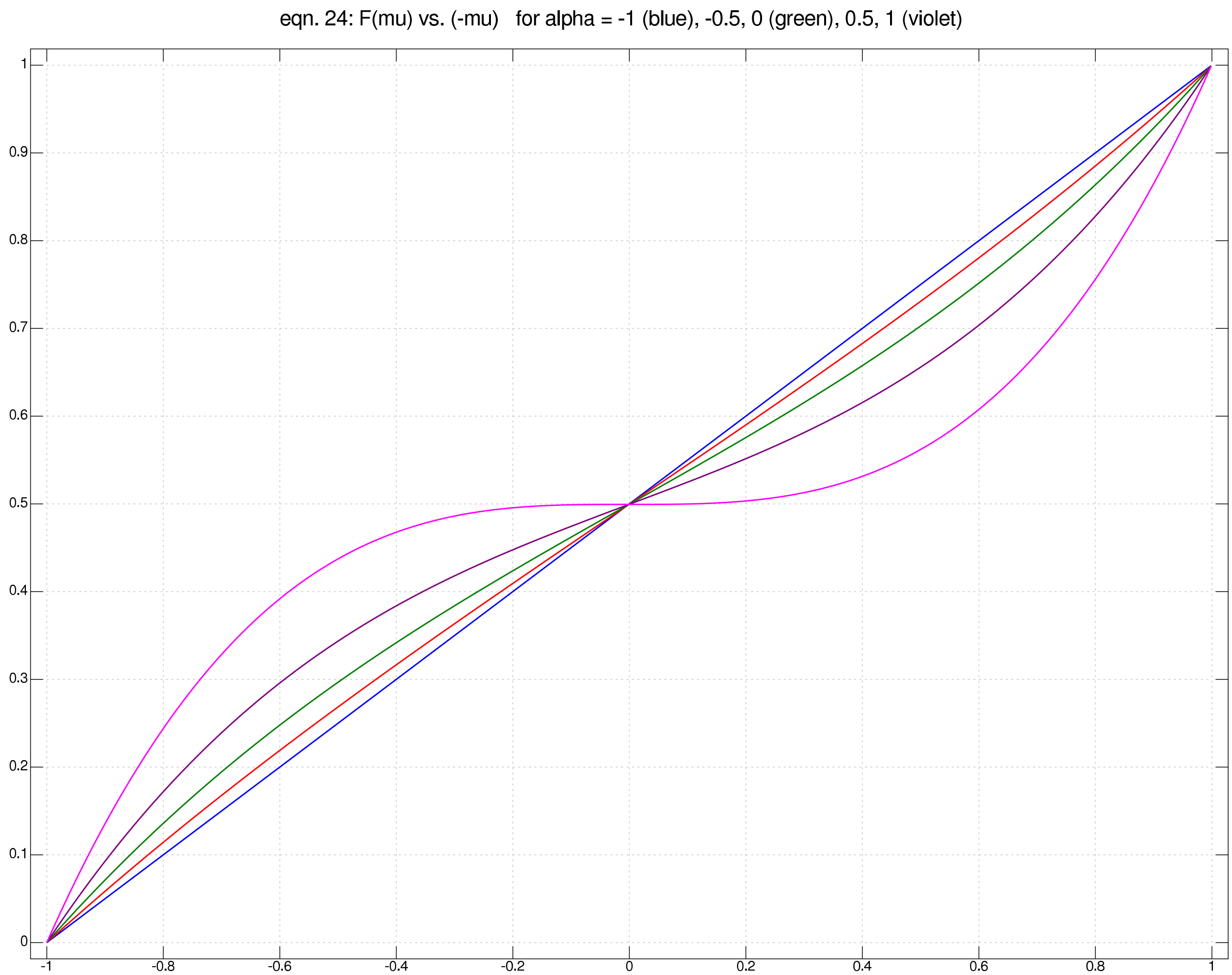

Fig. 6.— The cumulative function $F(\mu)$. (Plotted against $(-\mu)$ as $\mu = 1$ corresponds to $\theta = 0$.

$$\mu^3 \ + \ 3\left(\frac{1-\alpha}{1+\alpha}\right)\mu \ - \ \frac{2(2-\alpha)(1-2r)}{1+\alpha} \ = \ 0 \ . \tag{27}$$

The parameter α ranges over $-1 \leq \alpha \leq 1$. The value $\alpha = -1$ is a special case, for if we multiply eqn (24) by $(1+\alpha)$, we see that the cubic term vanishes and we have the solution

$$\mu \ = \ 1 - 2r \qquad \text{for the case} \qquad \alpha \ = \ -1 \ . \tag{28}$$

A value of $\alpha = -1$ will occur, for example, if the light is 100% linearly polarized perpendicular to the plane of scattering, so that $(Q_i/I_i) = -1$ for $\phi = 0$. Then the scattering will be independent of θ aside from the $\sin\theta$ from the differential of the spherical coordinate system. And indeed, eqn (26) is just a uniform distribution in $\mu = \cos\theta$ over [-1,1].

Another special case is $\alpha = 1$. This corresponds to 100% polarization in the plane of scattering. We see that then the coefficient of μ in eqn (24) vanishes and we have

$$\mu^3 \ - \ (1-2r) \ = \ 0 \quad \rightarrow \quad \mu \ = \ [1 \ - \ 2r]^{\frac{1}{3}} \ . \tag{29}$$

Another important case is unpolarized radiation, in which case $\alpha = 0$. Then eqn (24) becomes

$$\mu^3 \ + \ 3\mu \ - \ 2z \ = \ 0 \qquad \text{where} \qquad z \ = \ 2(1-2r) \ . \tag{30}$$

The only real solution to this cubic equation is

$$\mu \ = \ A + B \quad , \text{ where } \ A = \left[z + \sqrt{z^2+1}\right]^{\frac{1}{3}} \ \text{ and } \ B = \left[z - \sqrt{z^2+1}\right]^{\frac{1}{3}} \ . \tag{31}$$

The solution of eqn (24) for arbitrary α is not much more complex.

Let $z = (2-\alpha)(1-2r)$. Then we obtain

$$\mu \ = \ \frac{A+B}{(1+\alpha)^{\frac{1}{3}}} \ , \text{ where } \ A = \left[z + \sqrt{z^2 + \frac{(1-\alpha)^3}{(1+\alpha)}}\right]^{\frac{1}{3}} \ \text{ and } \ B = \left[z - \sqrt{z^2 + \frac{(1-\alpha)^3}{(1+\alpha)}}\right]^{\frac{1}{3}} \ . \tag{32}$$

Since the direct solution is a bit unwieldy, we might consider an iterative solution. If we call the l.h.s. of eqn (24) $f(\mu)$, the Newton-Raphson iterate $\mu_{n+1} = \mu_n - f(\mu)/(df/d\mu)$ is given by

$$\mu_{n+1} \ = \ \mu_n \ - \ \frac{(1+\alpha)\mu_n^3 + 3(1-\alpha)\mu_n - 2(2-\alpha)(1-2r)}{3\left[(1+\alpha)\mu_n^2 + (1-\alpha)\right]} \ . \tag{33}$$

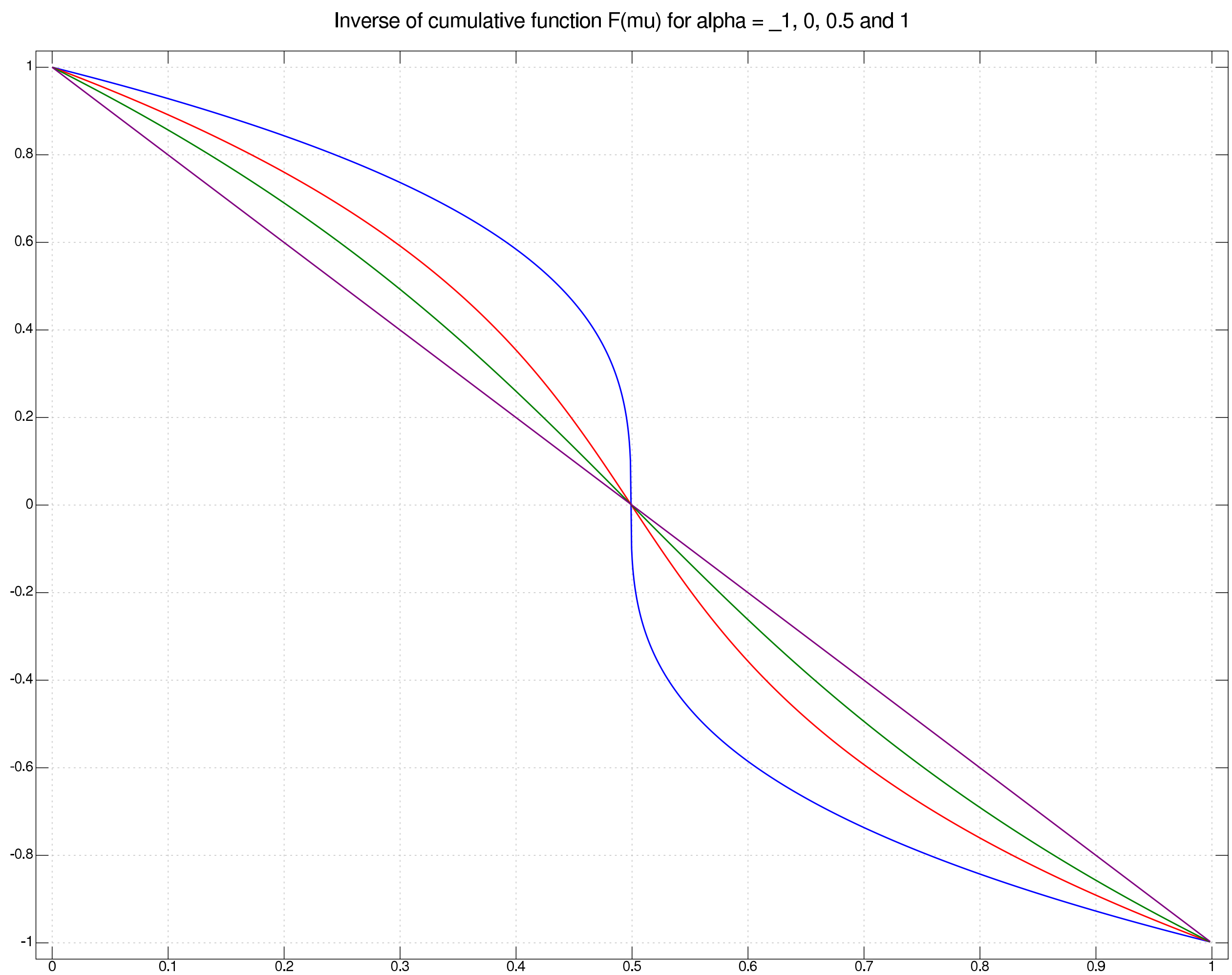

Fig. 7.— The inverse of the cumulative function $F(\mu)$. (The angle $\mu = \cos\theta$ plotted against F.) Plotted for $\alpha =$ -1, 0, 0.5, 1 (violet, green, red, blue).

Starting with $\mu_0 = r$, this converges well (less than 10 iterations) for $-1 \leq \alpha \leq 0.5$. However, as $\alpha \to 1$, more and more iterations are needed (e.g., 40 at $\alpha = 0.999999$, and over 600 at $\alpha = 1$).

4. Scattering by general non-aligned particles

A sufficiently general expression for the change of Stokes parameters under scattering by a collection on non-aligned particles is given by (Bohren & Huffman, p 413):

$$\begin{bmatrix} I_s \\ Q_s \\ U_s \\ V_s \end{bmatrix} = \begin{bmatrix} S_{11} & S_{12} & 0 & 0 \\ S_{12} & S_{22} & 0 & 0 \\ 0 & 0 & S_{33} & S_{34} \\ 0 & 0 & -S_{34} & S_{44} \end{bmatrix} \begin{bmatrix} I_i \\ Q_i \\ U_i \\ V_i \end{bmatrix} \tag{34}$$

The S_{ij} are of course functions of the scattering angle θ, and we exclude the case of particles with intrinsic optical activity, although linear birefringence and dichroism are permitted. If, further, we have isotropic spherical particles, then $S_{11} = S_{22}$ and $S_{33} = S_{44}$.

We might wonder why I_s is dependent on Q_i but has no dependence of U_i. Recall that U_i represents radiation polarized at an angle of 45^0 to the plane of scattering, and thus has equal intensities parallel and perpendicular to that plane. Thus the U_i intensity is equivalent to unpolarized radiation.

By analogy with equation (9) for the Rayleigh scattering case, the Stokes parameters of radiation scattered through angle θ in a scattering plane which makes an angle ϕ with respect to our reference axis is (referred to the plane of scattering)

$$\begin{bmatrix} I'_s \\ Q'_s \\ U'_s \\ V'_s \end{bmatrix} = \begin{bmatrix} S_{11}(\theta)I_i + S_{12}(\theta)(Q_i \cos 2\phi + U_i \sin 2\phi) \\ S_{12}(\theta)I_i + S_{22}(\theta)(Q_i \cos 2\phi + U_i \sin 2\phi) \\ S_{33}(\theta)(-Q_i \sin 2\phi + U_i \cos 2\phi) + S_{34}(\theta)V_i \\ S_{34}(\theta)(Q_i \sin 2\phi - U_i \cos 2\phi) + S_{44}(\theta)V_i \end{bmatrix} \tag{35}$$

To find the distribution of the scattered radiation as a function of ϕ, we can, as with Rayleigh scattering in § 3.1, integrate over all angles θ in the scattering plane. Let is define the averaged scattering elements as

$$\overline{S_{11}} = \frac{1}{2}\int_0^{\pi} S_{11}(\theta)\sin(\theta)d\theta = \frac{1}{2}\int_{-1}^{1} S_{11}(\mu)d\mu \quad \text{and} \quad \overline{S_{12}} = \frac{1}{2}\int_{-1}^{1} S_{12}(\mu)d\mu \tag{36}$$

where $\mu = \cos(\theta)$. We define $\overline{S_{22}}$, $\overline{S_{33}}$, $\overline{S_{34}}$, and $\overline{S_{44}}$ in the same way. As before, to combine Stokes parameters for different ϕ, we must rotate back to the original reference axis to obtain

$$\begin{bmatrix} \overline{I_s} \\ \overline{Q_s} \\ \overline{U_s} \\ \overline{V_s} \end{bmatrix} = \frac{1}{2\pi} \begin{bmatrix} I_i\ \overline{S_{11}}\ +\ (Q_i \cos 2\phi + U_i \sin 2\phi)\ \overline{S_{12}} \\ \cos 2\phi [I_i \overline{S_{12}} + (Q_i \cos 2\phi + U_i \sin 2\phi) \overline{S_{22}}] + \sin 2\phi [(Q_i \sin 2\phi - U_i \cos 2\phi) \overline{S_{33}} + V_i \overline{S_{34}}] \\ \sin 2\phi [I_i \overline{S_{12}} + (Q_i \cos 2\phi + U_i \sin 2\phi) \overline{S_{22}}] + \cos 2\phi [(-Q_i \sin 2\phi + U_i \cos 2\phi) \overline{S_{33}} + V_i \overline{S_{34}}] \\ (Q_i \sin 2\phi - U_i \cos 2\phi)\ \overline{S_{34}}\ +\ V_i\ \overline{S_{44}} \end{bmatrix} \tag{37}$$

The total scattered intensity then follows upon integration of $\overline{I_s}$ over ϕ:

$$\overline{\overline{I_s}} \ = \ \int_0^{2\pi} I_s d\phi \ = \ I_i\ \overline{S_{11}} \ + \ \frac{\overline{S_{12}}}{2\pi} \int_0^{2\pi} (Q_i \cos 2\phi + U_i \sin 2\phi)\ d\phi \ = \ I_i\ \overline{S_{11}} \tag{38}$$

where the second term vanishes since integrals of $\cos 2\phi$ and $\sin 2\phi$ over a multiple of π are zero. Thus to normalize the scattering matrix so that $\overline{\overline{I_s}} = I_i$, we must divide the elements by $\overline{S_{11}}$. From this point on, we will assume the scattering matrix has been properly normalized, such that

$$\overline{S_{11}} = \ \frac{1}{2} \int_0^{\pi} S_{11}(\theta) \sin(\theta) d\theta \ = \ \frac{1}{2} \int_{-1}^{1} S_{11}(\mu) d\mu \ = \ 1 \ \ . \tag{39}$$

(In the case of Rayleigh scattering, where $S_{11} = S_{22} = \frac{3}{4}(1+\mu^2)$, $S_{12} = -\frac{3}{4}(1-\mu^2)$, $S_{33} = S_{44} = \frac{3}{2}\mu$, and $S_{34} = 0$, we see that this normalization holds.)

Let us adopt lowercase for the Stokes parameters normalized by the incident intensity I_i : $q_i \equiv Q_i/I_i$, $u_i \equiv U_i/I_i$, $v_i \equiv V_i/I_i$, $i_s \equiv I_s/I_i$, etc. Then we see that equation (35) can be written equation (35) can be written

$$\begin{bmatrix} i'_s \\ q'_s \\ u'_s \\ v'_s \end{bmatrix} = \begin{bmatrix} S_{11}(\theta) + (q_i \cos 2\phi + u_i \sin 2\phi) S_{12}(\theta) \\ S_{12}(\theta) + (q_i \cos 2\phi + u_i \sin 2\phi) S_{22}(\theta) \\ (-q_i \sin 2\phi + u_i \cos 2\phi) S_{33}(\theta) + v_i S_{34}(\theta) \\ (q_i \sin 2\phi - u_i \cos 2\phi) S_{34}(\theta) + v_i S_{44}(\theta) \end{bmatrix} \tag{40}$$

Likewise, equation (37) can be written

$$\begin{bmatrix} \overline{i_s} \\ \overline{q_s} \\ \overline{u_s} \\ \overline{v_s} \end{bmatrix} = \frac{1}{2\pi} \begin{bmatrix} 1\ +\ (q_i \cos 2\phi + u_i \sin 2\phi)\ \overline{S_{12}} \\ \cos 2\phi [\overline{S_{12}} + (q_i \cos 2\phi + u_i \sin 2\phi) \overline{S_{22}}] + \sin 2\phi [(q_i \sin 2\phi - u_i \cos 2\phi) \overline{S_{33}} + v_i \overline{S_{34}}] \\ \sin 2\phi [\overline{S_{12}} + (q_i \cos 2\phi + u_i \sin 2\phi) \overline{S_{22}}] + \cos 2\phi [(-q_i \sin 2\phi + u_i \cos 2\phi) \overline{S_{33}} + v_i \overline{S_{34}}] \\ (q_i \sin 2\phi - u_i \cos 2\phi)\ \overline{S_{34}}\ +\ v_i\ \overline{S_{44}} \end{bmatrix} \tag{41}$$

If we then integrate over ϕ, as with equations (15) and (16), we see that

$$\begin{bmatrix} \overline{\overline{i_s}} \\ \overline{\overline{q_s}} \\ \overline{\overline{u_s}} \\ \overline{\overline{v_s}} \end{bmatrix} = \begin{bmatrix} 1 \\ \frac{1}{2}\ [\overline{S_{22}} + \overline{S_{33}}]\ q_i \\ \frac{1}{2}\ [\overline{S_{22}} + \overline{S_{33}}]\ u_i \\ \overline{S_{44}}\ v_i \end{bmatrix} \tag{42}$$

Since for Rayleigh scattering, $\overline{S_{22}} = 1$ while $\overline{S_{33}} = \overline{S_{44}} = 0$, this reduces to equation (16).

4.1. Distribution of ϕ angles.

We now generalize the treatment of §3.3 to this more general scattering matrix. We may assume we have rotated the reference axis to the plane of polarization of the incident beam. Then the normalized Stokes parameters will have the form $\{1, p_i, 0, v_i\}$. Then from eqn (41) we see that the intensity of the scattered radiation integrated over θ will be $\overline{i_s} = [1 + p_i\overline{S_{12}}\cos 2\phi]/2\pi$. (Note that $\overline{S_{12}}$ will generally be negative.) The cumulative distribution function $F(\phi)$ will then be

$$F(\phi) \ = \ \int_0^\phi \overline{i_s}(\phi')d\phi' \ = \ \frac{1}{2\pi}\int_0^\phi (1 + p_i\overline{S_{12}}\ \cos 2\phi')d\phi' \ = \ \frac{1}{2\pi}\left[\phi + \frac{1}{2}p_i\overline{S_{12}}\ \sin 2\phi\right] \ . \tag{43}$$

We see that $F(\phi)$ ranges over [0,1] as ϕ ranges from 0 to 2π, as it should. Now given that $F(\phi)$ is to be uniform over the interval [0,1], i.e., that $F(\phi)$ is represented by random numbers r over [0,1], to obtain the corresponding $\phi(r)$'s we must solve

$$4\pi r \ = \ 2\phi \ + \ p_i\overline{S_{12}}\ \sin 2\phi \ \ . \tag{44}$$

or, in the form of Kepler's equation,

$$M \ = \ E \ + \ p_i\overline{S_{12}}\ \sin E \ \ , \tag{45}$$

where $M = 4\pi\ r$, $E = 2\phi$, and the eccentricity is $p_i\overline{S_{12}}$. Recall that p_i is just the fractional *linear* polarization of the incident radiation. (For Rayleigh scattering, $\overline{S_{12}} = -1/2$ and we recover equation 23.) Again, we can solve this equation using a Newton-Raphson iteration:

$$E_{n+1} \ = \ E_n \ + \ \frac{(M - E_n) - p_i\overline{S_{12}}\ \sin E_n}{1 + p_i\overline{S_{12}}\ \cos E_n} \quad , \quad \text{with} \qquad E_0 \ = \ M \ \ . \tag{46}$$

So to find a uniform sampling of scattering angles ϕ', we get random values $M = 4\pi\ r$ for $0 \leq r \leq 1$, then solve eqn (45) for E, and our sample is $\phi' = E/2$. And again, since ϕ' is relative to the incoming plane of polarization, we we must add the angle of the polarization plane χ_i from eqn (5) to get the sampled angle relative to the reference plane: $\phi = \phi' + \chi_i$.

Another possible approach is to tabulate the solutions of (45) as a function of M and p_i , and use a 2-dimensional interpolation to find E.

4.2. Distribution of θ angles.

Let us suppose we have chosen a value of ϕ as outlined above. We now want to get a uniform sampling of θ, the scattering angle in the plane of scattering. From equation (40) we have $i'_s = S_{11}(\theta) + (q_i \cos 2\phi + u_i \sin 2\phi) S_{12}(\theta)$. With $\alpha = q_i \cos 2\phi + u_i \sin 2\phi$ and $\mu = \cos\theta$, the cumulative distribution has the form

$$\frac{1}{2}\int_0^\theta i'_s(\theta')\ \sin\theta'\ d\theta' \ = \ \frac{1}{2}\int_{-1}^{\mu} i'_s(\mu')\ d\mu' \ = \ \frac{1}{2}\int_{-1}^{\mu} S_{11}(\mu')\ d\mu' \ + \ \frac{\alpha}{2}\ \int_{-1}^{\mu} S_{12}(\mu')\ d\mu' \quad (47)$$

Integrating over [-1,1], we see that the normalization factor must be

$$\frac{1}{2}\int_{-1}^{1} S_{11}(\mu)\ d\mu \ + \ \frac{\alpha}{2}\ \int_{-1}^{1} S_{12}(\mu)\ d\mu \ = \ \overline{S_{11}} \ + \ \alpha\ \overline{S_{12}} \ = \ 1 \ + \ \alpha\ \overline{S_{12}} \quad (48)$$

thus the normalized cumulative distribution is given by

$$F(\mu) \ = \ \frac{1}{1+\alpha\overline{S_{12}}}\ \left\{ \frac{1}{2}\int_{-1}^{\mu} S_{11}(\mu')\ d\mu' \ + \ \frac{\alpha}{2}\int_{-1}^{\mu} S_{12}(\mu')\ d\mu' \right\} \ = \ \frac{\Sigma_{11}(\mu) \ + \ \alpha\ \Sigma_{12}(\mu)}{1+\alpha\overline{S_{12}}}\ , \quad (49)$$

where we have defined the integrated elements of the scattering matrix as

$$\Sigma_{11}(\mu) \ = \ \frac{1}{2}\int_{-1}^{\mu} S_{11}(\mu')\ d\mu' \quad \text{and} \quad \Sigma_{12}(\mu) \ = \ \frac{1}{2}\int_{-1}^{\mu} S_{12}(\mu')\ d\mu'\ . \quad (50)$$

Thus to obtain the angles $\theta = \arccos\mu$ for a Monte Carlo routine, we this need to solve the equation

$$(1+\alpha\overline{S_{12}})\ r \ = \ \Sigma_{11}(\mu) \ + \ \alpha\ \Sigma_{12}(\mu) \quad (51)$$

for μ , where r is a random number on the interval [0,1]. For any realistic scattering matrix, $S_{11}(\mu), S_{12}(\mu)$, etc. will result from numerical computations, and equation (51) must be solved numerically. For a given scattering matrix, we may compute $\overline{S_{12}}$, $\Sigma_{11}(\mu)$, and $\Sigma_{12}(\mu)$, and then compute a table of μ as a function of r and α.

5. Distribution of Scattering Angles by the Rejection Technique

Because the methods given above for obtaining the uniform sampling of the scattering angles θ and ϕ are complex, it is worthwhile to consider a statistical method which avoids the cumulative distribution function, the so-called *rejection technique* (von Neumann 1951). Consider the scattering phase function plotted over its full range, [0, 2π] for ϕ and [-1,1] for $\mu = \cos\theta$. Draw a horizontal line that is everywhere above this curve. Then we choose a *pair* of random numbers ξ_1 and ξ_2 that are uniformly distributed over this rectangular area, where ξ_1 represents the ϕ (or μ) coordinate, and ξ_2 the vertical (phase function) coordinate. If the point is below the curve, we accept ξ_1 as our sample, while if ξ_2 is above the curve at that ξ_1, we reject this pair and sample new (ξ_1, ξ_2) pairs until we succeed.

Consider the case of ϕ for Rayleigh scattering. The scattered intensity is given by $\overline{I_s} = [1 - \frac{1}{2}p\ \cos 2\phi]/2\pi$ (see equations (14) and (22)). We can thus consider the function $f(\phi) = 1 - \frac{1}{2}p\ \cos 2\phi$, which has an upper bound of $f_{max} = 1 + \frac{1}{2}p$. So we choose a pair of points r_1, r_2 both uniform over [0,1], so that $\xi_1 = 2\pi\ r_1$ and $\xi_2 = (1 + \frac{1}{2}p)\ r_2$, and ask if $\xi_2 \leq f(\xi_1)$, i.e.,

$$\text{If} \quad \left(1 + \frac{p}{2}\right)\ r_2\ \leq\ 1 - \frac{p}{2}\ \cos(4\pi\ r_1) \quad \text{then set} \quad \phi = 2\pi\ r_1\ , \quad \text{otherwise reject.} \qquad (52)$$

Fig. 8 shows the J code to get an array of ϕ's given an array of p's. Fetching 10^6 values takes less than a second.

We may find a uniform sample of μ's (and hence $\theta = \cos^{-1}(\mu)$) in the same manner. The phase function is $f(\mu) = (1 + \mu^2) - \alpha(1 - \mu^2)$ and $f_{max} = 2$ (§3.4) so if we take $\xi_1 = 2r_1 - 1$ and $\xi_2 = 2r_2$, the test $\xi_2 \leq f(\xi_1)$ becomes, for a pair (r_1, r_2) uniform over [0,1],

$$\text{If} \quad 2\,r_2\ \leq\ [1{+}(2r_1{-}1)^2]{-}\alpha[1{-}(2r_1{-}1)^2] \quad \text{then set} \quad \mu = 2r_1{-}1\ , \quad \text{otherwise reject.} \qquad (53)$$

For the more general scattering matrix considered in §4, we have from §4.1 the phase function $f(\phi) = 1 + \overline{S_{12}}\ p\ \ \cos 2\phi$, which leads to the rejection condition

$$\text{If} \quad \left(1 + |\overline{S_{12}}|\ p\right)\ r_2\ \leq\ 1{+}\overline{S_{12}}\,p\ \cos(4\pi\,r_1) \quad \text{then set} \quad \phi = 2\pi\,r_1\ , \quad \text{otherwise reject.} \qquad (54)$$

Likewise, the more general expression for μ follows from §4.2, where we see that the phase function is $f(\mu) = S_{11}(\mu) + \alpha S_{12}(\mu)$. Now we need to know f_{max}, the maximum value of $f(\mu)$ over the interval $-1 \leq \mu \leq 1$. The parameter $\alpha = q_i \cos 2\phi + u_i \sin 2\phi$ can take any value over the range $-1 \leq \alpha \leq 1$. With a detailed knowledge of $S_{11}(\mu)$ and $S_{12}(\mu)$, we can evaluate $f_{max}(\alpha)$. Then the rejection condition for μ becomes

$$\text{If} \quad f_{max}(\alpha)\ r_2\ \leq\ S_{11}(2r_1 - 1) + \alpha S_{12}(2r_1 - 1) \quad \text{then} \quad \mu = 2r_1 - 1\ , \quad \text{otherwise reject.} \qquad (55)$$

A problem may arise if $S_{11}(\mu)$ and/or $S_{12}(\mu)$ has a strong peak, e.g. Mie scattering by large particles in the forward direction ($\mu = 1$). Then over other values of μ, our $[\xi_1, \xi_2]$ pairs will be strongly rejected, and excessive re-sampling will occur.

6. References.

Bohren, C.F., and Huffman, D.R. 1983,"Absorption and Scattering of Light by Small Particles", (John Wiley & Sons, New York).

Hovenier, J.W., van der Mee, C. and Domke, H. 2004, "Transfer of Polarized Light in Planetary Atmospheres: Basic Concepts and Practical Methods", (Kluwer, Dordrecht)

Mishchenko, M.I., Travis, L.D. and Lacis, A.A. 2002, "Scattering, Absorption, and Emission of Light by Small Particles", (Cambridge University Press, Cambridge, UK)
The entire book (revised edition) is available as a free *.pdf* download from
http://www.giss.nasa.gov/staff/mmishchenko/books.html

van de Hulst, H.C. 1981,"Light Scattering by Small Particles"(Dover Pub., NY), a reprint of the original 1957 edition.

von Neumann, J. 1951,"Various techniques used in connection with random digits", *National Bureau of Standards Applied Mathematics Series*, **12**, 36.

```
NB. Find phi' angles for various polarizations "p" for
NB. Rayleigh scattering, using the rejection technique.
NB. Usage: rj-PHI p --> phi'
rj_PHI=: 3 : 0
inr=. I. bi=. (n=. #y)#1   NB. inr are indices still to do
phip=. n#0                 NB. placeholder for phi' results
while. n>0 do.
  r=. 2p1* rand n          NB. trial value of phi'
  b2=: (inr{y) p_test r    NB. call the test function
  inn=. I. b2              NB. subarray index of those which pass
  idx=. inn{inr            NB. corresponding index in whole array
  phip=. (inn{r) idx}phip  NB. insert successful phi's
  inr=. I. bi=. 0 idx} bi  NB. remove those done from inr
  n=. +/bi                 NB. number left to do
end. phip
)
NB. Is r2*(1+p/2) <= 1 - (p/2)cos(2*r1) ?
p_test=: 4 : '((1+ -:x)*(rand #y))<: 1- -:x*cos +:y'
```

Fig. 8.— J code for finding ϕ by rejection technique.