Rehr-Albers Approximation to Electron Diffraction - V 4.0

References:

[1] J. J. Rehr and R. C. Albers, PRB **41**, 8139 (1990);
[2] A. P. Kaduwela, D. J. Friedman and C. S. Fadley, J. Elect. Spect. and Rel. Phenom., **57**, 223 (1991);
[3] J. Mustre de Leon, J. J. Rehr, S. I. Zabinsky, and R. C. Albers, PRB **44**, 4146 (1991).

This file contains function definitions for use with calculations using the R-A approximation to electron diffraction. Embed this document into your working calculation.

Version 2.0, July 19, 97 -- Created DLLs for rotm, ctos and stoc, obviating need for explicit definitions.

Version 3.0, August 4, 98 -- Moved definitions of introduction matrix, termination matrix and refraction through inner potential to this file.

Function definitions:

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Spherical harmonic normalization factors: for use in calculating γ and γt.

$$\mathrm{NLM}(l,\mu) := \begin{cases} 0 & \text{if } \mu > l \\ \sqrt{\dfrac{(2\cdot l+1)\cdot(l-\mu)!}{(l+\mu)!}} & \text{otherwise} \end{cases}$$

Appears OK, 12/22/95.
Modified 3/3/97 to require μ <= l.

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Dimensionless polynomial factor which multiplies the asymptotic form of the spherical Hankel function:

$$c(l,z) := \sum_{s=0}^{l} \frac{1}{2^s\cdot s!}\cdot\frac{(l+s)!}{(l-s)!}\cdot(-z)^s$$

3/3/97, replaced with alternate series form. Still blows up for large z,l.

Tested again 4/28/97. Series form is exactly equivalent to the recursive form. c(0,z) = 1 all z.

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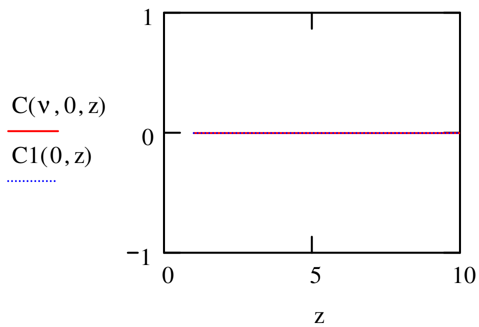
C-function, derivative of the polynomial part of the spherical Hankel function. Only ν = 0, 1, and 2 are ever used in a Rehr-Albers calculation. Since the zeroth derivative is just c(l,z), only the first and second need to be defined. Analytical expressions based on the series expansion work very well, compared to the numerical derivative.

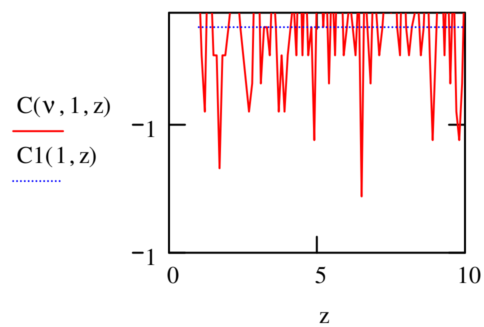
$$C(\nu,l,z) := \frac{d^\nu}{dz^\nu}c(l,z)$$

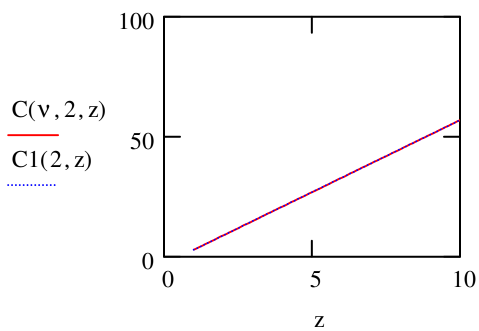
Checked OK 12/22/95

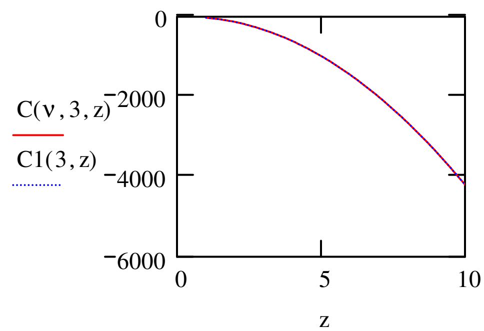
$$C1(L,z) := \sum_{s=0} \frac{(-s)}{2^s \cdot s!} \cdot \frac{L+s!}{L-s!} \cdot (-z)^{s-1} \qquad C2(L,z) := \sum_{s=0} \frac{s\cdot(s-1)}{2^s \cdot s!} \cdot \frac{L+s!}{L-s!} \cdot (-z)^{s-2}$$

$$z := 1, 1.1 .. 10 \quad \nu := 1$$









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Spherical expansion coefficients g and g-twiddle (denoted gt) (ref. [1], Eq. 12). L is a vector with two elements L=(l,m), l is a vector with two elements l=(m,n), r is a dimensionless "bond length" scalar = kr.

$$\gamma(L,\lambda,\rho) := (-1)^{|\lambda_0|} \cdot NLM\left(L_0, |\lambda_0|\right) \cdot \frac{C\left(|\lambda_0| + \lambda_1, L_0, \frac{1}{i\cdot\rho}\right)}{|\lambda_0| + \lambda_1!} \cdot \left[\left(\frac{1}{i\cdot\rho}\right)^{|\lambda_0|+\lambda_1}\right]$$

Test values:

$$\gamma\left[\begin{pmatrix}0\\0\end{pmatrix}, \begin{pmatrix}0\\0\end{pmatrix}, 1\right] = 1$$

= 1, independent of r.

$$\gamma\left[\begin{pmatrix}2\\0\end{pmatrix}, \begin{pmatrix}1\\0\end{pmatrix}, 10\right] = 0.05477 - 0.27386i$$

= 0.05477 - 0.27386i.

Checks out OK, 12/22/95. Above test values calculated from formulas by hand, and entered 3/3/97. Note - second test fails if we substitute approximate form for C(l,n,r).

$$(2\cdot L_0 + 1) \quad C\left(\lambda_1, L_0, \frac{1}{i\cdot\rho}\right) \quad \left(\frac{1}{\ }\right)^{\lambda_1}$$

$$\gamma t(L,\lambda,\rho) := \frac{\left(\quad 0 \quad\right)}{NLM\left(L_0, \left|\lambda_0\right|\right)} \cdot \frac{\left(\quad i\cdot\rho \right)}{\lambda_1 !} \cdot \left(\frac{1}{i\cdot\rho}\right)$$

Test values:

$$\gamma t\left[\begin{pmatrix}0\\0\end{pmatrix},\begin{pmatrix}0\\0\end{pmatrix},1\right] = 1$$

= 1, independent of r.

$$\gamma t\left[\begin{pmatrix}2\\0\end{pmatrix},\begin{pmatrix}1\\0\end{pmatrix},10\right] = 5.31291 + 1.64317i$$

= 5.31291 + 1.64317i.

Checks out OK, 12/22/95. Above test values calculated from formulas by hand, and entered 3/3/97.
Note - second test fails if we substitute approximate form for C(l,n,r), but not as badly as g.

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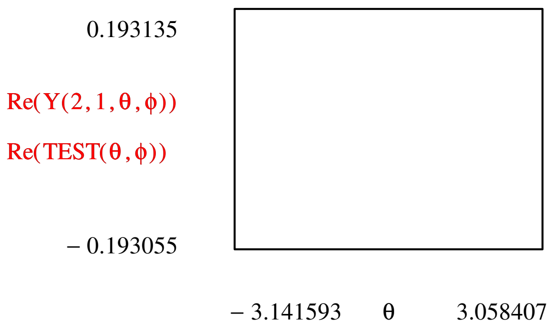
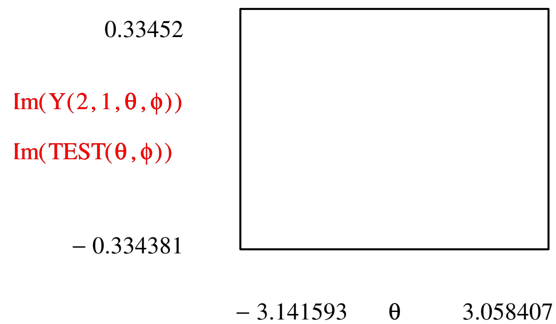
Define the spherical harmonics $Y_{lm}(\theta,\phi)$
Have to account explicitly for the case where m is odd and sin(q) is < 0. The square root in the plgndr() routine only returns the +ve root - in cases where we want the -ve root, we have to add it in explicitly.

$$Y(l,m,\theta,\phi) := \left|\begin{array}{l} y \leftarrow \frac{1}{\sqrt{4\cdot\pi}}\cdot NLM(l,|m|)\cdot plgndr(l,|m|,\cos(\theta))\cdot\left(e^{i\cdot m\cdot\phi}\right) \\ \left[y \leftarrow (-1)^m\cdot y\right] \text{ if } (m \ge 0) \\ \left[y \leftarrow (-1)^m\cdot y\right] \text{ if } \sin(\theta) > 0 \\ y \end{array}\right.$$

Tested OK for l <= 2, 3/4/97.

$$TEST(\theta,\phi) := -\sqrt{\frac{15}{8\cdot\pi}}\cdot\sin(\theta)\cdot\cos(\theta)\cdot\exp(i\cdot\phi) \qquad \theta := -\pi, -\pi + 0.1 .. \pi \qquad \phi := \frac{\pi}{3}$$





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Spherical rotation matrices, per Messiah, p. 1072.

rotm() was moved to a DLL, 7/19/97. Checks out OK.

Test values:

$$\text{test1}(\beta) := \begin{bmatrix} \frac{1}{2}\cdot(1+\cos(\beta)) & -\frac{1}{\sqrt{2}}\cdot\sin(\beta) & \frac{1}{2}\cdot(1-\cos(\beta)) \\ \frac{1}{\sqrt{2}}\cdot\sin(\beta) & \cos(\beta) & -\frac{1}{\sqrt{2}}\cdot\sin(\beta) \\ \frac{1}{2}\cdot(1-\cos(\beta)) & \frac{1}{\sqrt{2}}\cdot\sin(\beta) & \frac{1}{2}\cdot(1+\cos(\beta)) \end{bmatrix}$$

Special case for J=1. Successive rows correspond to M = +1, 0, -1; the columns are arranged in the same order from left to right.

$$\text{test2}(\beta) := \begin{pmatrix} \text{rotm}(1,1,1,\beta) & \text{rotm}(1,1,0,\beta) & \text{rotm}(1,1,-1,\beta) \\ \text{rotm}(1,0,1,\beta) & \text{rotm}(1,0,0,\beta) & \text{rotm}(1,0,-1,\beta) \\ \text{rotm}(1,-1,1,\beta) & \text{rotm}(1,-1,0,\beta) & \text{rotm}(1,-1,-1,\beta) \end{pmatrix}$$

Same array calculated with rotm().

$$\text{test1}(0.25) = \begin{pmatrix} 0.98446 & -0.17494 & 0.01554 \\ 0.17494 & 0.96891 & -0.17494 \\ 0.01554 & 0.17494 & 0.98446 \end{pmatrix} \qquad \text{test1}(1) = \begin{pmatrix} 0.77015 & -0.59501 & 0.22985 \\ 0.59501 & 0.5403 & -0.59501 \\ 0.22985 & 0.59501 & 0.77015 \end{pmatrix}$$

$$\text{test2}(0.25) = \begin{pmatrix} 0.98446 & -0.17494 & 0.01554 \\ 0.17494 & 0.96891 & -0.17494 \\ 0.01554 & 0.17494 & 0.98446 \end{pmatrix} \qquad \text{test2}(1) = \begin{pmatrix} 0.77015 & -0.59501 & 0.22985 \\ 0.59501 & 0.5403 & -0.59501 \\ 0.22985 & 0.59501 & 0.77015 \end{pmatrix}$$

Checks out OK, 7/19/97.

Check symmetry relation rotm(J,M,M',b) = rotm(J,M',M,-b).

$J := 2 \quad M := 2 \quad M' := -1 \quad \beta := 1.517$

$$\text{rotm}(J,M,M',\beta) = -0.47243$$
$$\text{rotm}(J,M',M,-\beta) = -0.47243$$

Should be equal. Checks OK 7/19/97.

Special case for j=1/2. Successive lines correspond to M=1/2, -1/2; the columns are arranged in the same order from left to right.

$$\text{test1}(\beta) := \begin{pmatrix} \cos\left(\frac{\beta}{2}\right) & -\sin\left(\frac{\beta}{2}\right) \\ \sin\left(\frac{\beta}{2}\right) & \cos\left(\frac{\beta}{2}\right) \end{pmatrix} \quad \text{test2}(\beta) := \begin{pmatrix} \text{rotm}\left(\frac{1}{2},\frac{1}{2},\frac{1}{2},\beta\right) & \text{rotm}\left(\frac{1}{2},\frac{1}{2},\frac{-1}{2},\beta\right) \\ \text{rotm}\left(\frac{1}{2},\frac{-1}{2},\frac{1}{2},\beta\right) & \text{rotm}\left(\frac{1}{2},\frac{-1}{2},\frac{-1}{2},\beta\right) \end{pmatrix}$$

$$\text{test1}(1) = \begin{pmatrix} 0.87758 & -0.47943 \\ 0.47943 & 0.87758 \end{pmatrix}$$

Checks out OK, 7/19/97.

$$\text{test2}(1) = \begin{pmatrix} 0.87758 & -0.47943 \\ 0.47943 & 0.87758 \end{pmatrix}$$

Test special case where J is integral, and M' = J.

$$\mathrm{test}(L,M,\beta) := \sqrt{\frac{2\cdot L!}{L+M!\cdot L-M!}}\cdot\frac{1}{2^L}\cdot(1+\cos(\beta))^M\cdot\sin(\beta)^{L-M}$$

$L := 2 \quad M := -1 \quad \beta := -1.2823$

$\mathrm{rotm}(L,M,L,\beta) = -0.34296$ Checks out OK, 7/19/97.

$\mathrm{test}(L,M,\beta) = -0.34296$

Define the capital R rotation matrix.

$$\mathrm{ROTM}(J,M,M',\alpha,\beta,\gamma) := \exp(-i\cdot\alpha\cdot M)\cdot\mathrm{rotm}(J,M,M',\beta)\cdot\exp(-i\cdot\gamma\cdot M')$$

Test values: check orthonormality.

$$\mathrm{DelM}(J,M',M'',\alpha,\beta,\gamma) := \sum_{M=-J}^{J}\mathrm{ROTM}(J,M,M',\alpha,\beta,\gamma)\cdot\overline{\mathrm{ROTM}(J,M,M'',\alpha,\beta,\gamma)}$$

$\mathrm{DelM}(2,2,1,0.1,0.2,0.3) = 0$

$\mathrm{DelM}(2,2,2,0.1,0.2,0.3) = 1$ Should = 0 unless M' = M''.

Seems to check out OK, 3/3/97.

Check special cases where M or M' are zero:

$$\mathrm{TEST1}(L,M,\alpha,\beta,\gamma) := \sqrt{\frac{4\cdot\pi}{2\cdot L+1}}\cdot\overline{Y(L,M,\beta,\alpha)}$$

$L := 2 \quad M := -1 \quad \alpha := 8.5 \quad \beta := -.7 \quad g := 2.5$

$\mathrm{TEST1}(L,M,\alpha,\beta,g) = ▮$

$\mathrm{ROTM}(L,M,0,\alpha,\beta,g) = 0.36329 - 0.48186i$

Checks out OK, 6/10/97.

$$\mathrm{TEST1}(L,M,\alpha,\beta,\gamma) := \sqrt{\frac{4\cdot\pi}{2\cdot L+1}}\cdot\overline{Y(L,M,\beta,\gamma)}\cdot(-1)^M$$

$L := 2 \quad M := -1 \quad \alpha := 0.5 \quad \beta := -5.7 \quad g := -9.5$

$\mathrm{TEST1}(L, M, \alpha, \beta, g) = \blacksquare$

$\mathrm{ROTM}(L, 0, M, \alpha, \beta, g) = 0.56138 - 0.04231i$

Checks out OK, 6/10/97.

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Define G and G-twiddle per ref. [1], Eq. 13. r is a vector, in spherical coordinates.

$$\Gamma(L, \lambda, \rho) := \left| \begin{array}{l} \alpha \leftarrow 0 \\ \beta \leftarrow \rho_1 \\ g \leftarrow \pi - \rho_2 \\ \mathrm{ROTM}(L_0, \lambda_0, L_1, \alpha, \beta, g) \cdot \gamma(L, \lambda, \rho_0) \end{array} \right.$$

$$\Gamma t(L, \lambda, \rho) := \left| \begin{array}{l} \alpha \leftarrow 0 \\ \beta \leftarrow \rho_1 \\ g \leftarrow \pi - \rho_2 \\ \mathrm{ROTM}(L_0, L_1, \lambda_0, -g, -\beta, -\alpha) \cdot \gamma t(L, \lambda, \rho_0) \end{array} \right.$$

Test values: $\rho := \begin{pmatrix} 10 \\ \frac{\pi}{7} \\ \frac{\pi}{3} \end{pmatrix} \quad L := \begin{pmatrix} 4 \\ 3 \end{pmatrix}$

$\mathrm{TEST1}(L) := \sqrt{4 \cdot \pi} \cdot Y(L_0, L_1, \rho_1, \rho_2) \cdot c\left(L_0, \frac{1}{i \cdot \rho_0}\right)$ Should be = to G(L,0,r)

$\mathrm{TEST2}(L) := \sqrt{4 \cdot \pi} \cdot \overline{Y(L_0, L_1, \rho_1, \rho_2)} \cdot c\left(L_0, \frac{1}{i \cdot \rho_0}\right)$ Should be = to Gt(L,0,r)

$\mathrm{TEST1}(L) = \blacksquare$

$\Gamma\left[L, \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \rho\right] = 0.18302 + 0.29225i$

$\mathrm{TEST2}(L) = \blacksquare$

$\Gamma t\left[L, \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \rho\right] = 0.18302 + 0.29225i$

Checks out OK, 3/4/97.

$$\Gamma\left[\begin{pmatrix}2\\1\end{pmatrix},\begin{pmatrix}1\\0\end{pmatrix},\rho\right] = -0.20165 + 0.06822i$$

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C_to_S(v): converts the vector v, which is in cartesian coordinates, to a vector s, which is in spherical coordinates.
S_to_C(s): converts the vector s, which is in spherical coordinates, to a vector v, which is in cartesian coordinates.

Replaced 7/19/97 with ctos() and stoc(), compiled in DLLs.

Test values:

$$V := \begin{pmatrix}-2.6\\-10.2\\3.2\end{pmatrix} \qquad \mathrm{ctos}(V) = \begin{pmatrix}11.00182\\1.27567\\4.4628\end{pmatrix} \qquad \mathrm{stoc}(\mathrm{ctos}(V)) = \begin{pmatrix}-2.6\\-10.2\\3.2\end{pmatrix}$$

Checks out OK, 7/19/97.

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"Scattering Matrix" $F(\lambda,\lambda',\rho,\rho',t)$:

- λ,λ' - two-element matrices $\lambda=(\mu,\nu)$.
- ρ,ρ' - vectors defined as $k(\mathbf{r}-\mathbf{R})$, in spherical coordinates.
- t - t-matrix of atom at **R**. $t = \exp(i\delta_l)\sin(\delta_l)$, has LMAX elements.

*** DAH-AN -- this routine has a sign error somewhere, which is apparent if you look at the test values below. Since the scattering matrix is used for double scattering or higher, it isn't needed for single scattering. Still, if you can find the error, you win a cookie.

Seems to be an error in this routine: If $\mu + \mu'$ is odd, an overall minus sign appears. Either I'm doing something wrong, or Rehr's putting something into the routine which ought not be there.

$$F(\lambda,\lambda',\rho,\rho',t) := \left| \begin{array}{l} NL \leftarrow \mathrm{rows}(t) - 1 \\ f \leftarrow \displaystyle\sum_{l=0}^{NL} \sum_{m=-l}^{l} \Gamma\left[\begin{pmatrix}l\\m\end{pmatrix},\lambda,\rho\right]\cdot\Gamma t\left[\begin{pmatrix}l\\m\end{pmatrix},\lambda',\rho'\right]\cdot t_l \\ f \end{array}\right.$$

Test values: generated by Greg Schenter for Si cluster from FEFF 7.0. Note that the notation reads ρ' is the vector going *into* the scattering event, and ρ is the vector going *away* from the scatterer.

$$\delta := \begin{pmatrix} -.4004146 \\ .6112068 \\ 1.329133 \\ 3.146167\cdot 10^{-1} \\ 4.819505\cdot 10^{-2} \\ 5.902354\cdot 10^{-3} \\ 5.629561\cdot 10^{-4} \\ 4.174712\cdot 10^{-5} \\ 2.449426\cdot 10^{-6} \\ 1.161656\cdot 10^{-7} \\ 0 \end{pmatrix}$$

<-- Test phase shifts.

$k := 1.8842$

$$TM := \overrightarrow{\exp(i\cdot\delta)\cdot\sin(\delta)}$$

T-matrix, from phase shifts.

$$\rho := \mathrm{ctos}\left[\begin{pmatrix} 0 \\ 0 \\ 7.5589 \end{pmatrix}\cdot k\right] \qquad \rho' := \mathrm{ctos}\left[\begin{pmatrix} 2.5653 \\ -2.5653 \\ 2.5653 \end{pmatrix}\cdot k\right]$$

Define ρ, ρ'.

$$\rho = \begin{pmatrix} 14.24248 \\ 0 \\ 0 \end{pmatrix} \qquad \rho' = \begin{pmatrix} 8.37193 \\ 0.95532 \\ -0.7854 \end{pmatrix}$$

Test values for all possible values of λ, λ'.

Function definition above: Rehr's code

Function definition above	Rehr's code
$F\left[\begin{pmatrix} 0 \\ 0 \end{pmatrix},\begin{pmatrix} 0 \\ 0 \end{pmatrix},\rho,\rho',TM\right] = 0.3192 - 0.18499i$	= 0.319210 - 0.184990 i
$F\left[\begin{pmatrix} 0 \\ 0 \end{pmatrix},\begin{pmatrix} -1 \\ 0 \end{pmatrix},\rho,\rho',TM\right] = -0.76349 + 9.20784i$	= 0.763540 - 9.20780 i
$F\left[\begin{pmatrix} 0 \\ 0 \end{pmatrix},\begin{pmatrix} 1 \\ 0 \end{pmatrix},\rho,\rho',TM\right] = 0.76349 - 9.20784i$	=-0.763540 + 9.20780 i
$F\left[\begin{pmatrix} 0 \\ 0 \end{pmatrix},\begin{pmatrix} 0 \\ 1 \end{pmatrix},\rho,\rho',TM\right] = 0.79725 + 3.68122i\times 10^{-3}$	= 0.797260 + 3.69130E-03 i
$F\left[\begin{pmatrix} 0 \\ 0 \end{pmatrix},\begin{pmatrix} -2 \\ 0 \end{pmatrix},\rho,\rho',TM\right] = -2.91224 + 25.73973i$	= -2.9125 + 25.7400 i
$F\left[\begin{pmatrix} 0 \\ 0 \end{pmatrix},\begin{pmatrix} 2 \\ 0 \end{pmatrix},\rho,\rho',TM\right] = -2.91224 + 25.73973i$	= -2.9125 + 25.7400 i
$F\left[\begin{pmatrix} -1 \\ 0 \end{pmatrix},\begin{pmatrix} 0 \\ 0 \end{pmatrix},\rho,\rho',TM\right] = -0.23244 + 0.22735i$	= 0.232440 - 0.227349 i
$F\left[\begin{pmatrix} -1 \\ 0 \end{pmatrix},\begin{pmatrix} -1 \\ 0 \end{pmatrix},\rho,\rho',TM\right] = -0.2246 + 0.1827i$	= -0.224600 + 0.182693 i

$$F\left[\begin{pmatrix}-1\\0\end{pmatrix},\begin{pmatrix}1\\0\end{pmatrix},\rho,\rho',TM\right] = 0.79395 - 0.73959i$$ = 0.793974 - 0.739599 i

$$F\left[\begin{pmatrix}-1\\0\end{pmatrix},\begin{pmatrix}0\\1\end{pmatrix},\rho,\rho',TM\right] = -0.09939 - 0.06743i$$ = 0.0993903 + 0.0674302 i

$$F\left[\begin{pmatrix}-1\\0\end{pmatrix},\begin{pmatrix}-2\\0\end{pmatrix},\rho,\rho',TM\right] = 1.57416 - 1.68371i$$ = -1.57419 + 1.68373 i

$$F\left[\begin{pmatrix}-1\\0\end{pmatrix},\begin{pmatrix}2\\0\end{pmatrix},\rho,\rho',TM\right] = -1.72596 + 1.36298i$$ = 1.72597 - 1.36296 i

$$F\left[\begin{pmatrix}1\\0\end{pmatrix},\begin{pmatrix}0\\0\end{pmatrix},\rho,\rho',TM\right] = 0.22735 + 0.23244i$$ = -0.227349 - 0.232441 i

$$F\left[\begin{pmatrix}1\\0\end{pmatrix},\begin{pmatrix}-1\\0\end{pmatrix},\rho,\rho',TM\right] = 0.73959 + 0.79395i$$ = 0.739596 + 0.793977 i

$$F\left[\begin{pmatrix}1\\0\end{pmatrix},\begin{pmatrix}1\\0\end{pmatrix},\rho,\rho',TM\right] = -0.1827 - 0.2246i$$ = -0.182693 - 0.224601 i

$$F\left[\begin{pmatrix}1\\0\end{pmatrix},\begin{pmatrix}0\\1\end{pmatrix},\rho,\rho',TM\right] = -0.06743 + 0.09939i$$ = 0.0674306 - 0.0993901 i

$$F\left[\begin{pmatrix}1\\0\end{pmatrix},\begin{pmatrix}-2\\0\end{pmatrix},\rho,\rho',TM\right] = 1.36298 + 1.72596i$$ = -1.36295 - 1.72597 i

$$F\left[\begin{pmatrix}1\\0\end{pmatrix},\begin{pmatrix}2\\0\end{pmatrix},\rho,\rho',TM\right] = -1.68371 - 1.57416i$$ = 1.68373 + 1.57420 i

$$F\left[\begin{pmatrix}0\\1\end{pmatrix},\begin{pmatrix}0\\0\end{pmatrix},\rho,\rho',TM\right] = 0.45629 + 0.03149i$$ = 0.456300 + 0.0314970 i

$$F\left[\begin{pmatrix}0\\1\end{pmatrix},\begin{pmatrix}-1\\0\end{pmatrix},\rho,\rho',TM\right] = -2.0055 + 0.10814i$$ = 2.00550 - 0.108130 i

$$F\left[\begin{pmatrix}0\\1\end{pmatrix},\begin{pmatrix}1\\0\end{pmatrix},\rho,\rho',TM\right] = 2.0055 - 0.10814i$$ = -2.00550 + 0.108130 i

$$F\left[\begin{pmatrix}0\\1\end{pmatrix},\begin{pmatrix}0\\1\end{pmatrix},\rho,\rho',TM\right] = 0.04139 + 0.44067i$$ = 0.0413860 + 0.440680 i

$$F\left[\begin{pmatrix}0\\1\end{pmatrix},\begin{pmatrix}-2\\0\end{pmatrix},\rho,\rho',TM\right] = -9.93859 - 0.1383i$$ = -9.93870 - 0.138410 i

$$F\left[\begin{pmatrix}0\\1\end{pmatrix},\begin{pmatrix}2\\0\end{pmatrix},\rho,\rho',TM\right] = -9.93859 - 0.1383i$$ = -9.93870 - 0.138410 i

$$F\left[\begin{pmatrix}-2\\0\end{pmatrix},\begin{pmatrix}0\\0\end{pmatrix},\rho,\rho',TM\right] = -0.01594 + 1.63045i \times 10^{-3}$$

$$F\left[\begin{pmatrix}-2\\0\end{pmatrix},\begin{pmatrix}-1\\0\end{pmatrix},\rho,\rho',TM\right] = 0.03949 - 7.06409i \times 10^{-3}$$

$$F\left[\begin{pmatrix}-2\\0\end{pmatrix},\begin{pmatrix}1\\0\end{pmatrix},\rho,\rho',TM\right] = 0.0386 - 9.23444i \times 10^{-4}$$

$$F\left[\begin{pmatrix}-2\\0\end{pmatrix},\begin{pmatrix}0\\1\end{pmatrix},\rho,\rho',TM\right] = -2.78516 \times 10^{-3} - 0.01036i$$

$$F\left[\begin{pmatrix}-2\\0\end{pmatrix},\begin{pmatrix}-2\\0\end{pmatrix},\rho,\rho',TM\right] = 0.03511 + 2.29438i \times 10^{-3}$$

$$F\left[\begin{pmatrix}-2\\0\end{pmatrix},\begin{pmatrix}2\\0\end{pmatrix},\rho,\rho',TM\right] = -0.07093 - 0.01649i$$

$$F\left[\begin{pmatrix}2\\0\end{pmatrix},\begin{pmatrix}0\\0\end{pmatrix},\rho,\rho',TM\right] = 0.01594 - 1.63045i \times 10^{-3}$$

$$F\left[\begin{pmatrix}2\\0\end{pmatrix},\begin{pmatrix}-1\\0\end{pmatrix},\rho,\rho',TM\right] = 0.0386 - 9.23444i \times 10^{-4}$$

$$F\left[\begin{pmatrix}2\\0\end{pmatrix},\begin{pmatrix}1\\0\end{pmatrix},\rho,\rho',TM\right] = 0.03949 - 7.06409i \times 10^{-3}$$

$$F\left[\begin{pmatrix}2\\0\end{pmatrix},\begin{pmatrix}0\\1\end{pmatrix},\rho,\rho',TM\right] = 2.78516 \times 10^{-3} + 0.01036i$$

$$F\left[\begin{pmatrix}2\\0\end{pmatrix},\begin{pmatrix}-2\\0\end{pmatrix},\rho,\rho',TM\right] = 0.07093 + 0.01649i$$

$$F\left[\begin{pmatrix}2\\0\end{pmatrix},\begin{pmatrix}2\\0\end{pmatrix},\rho,\rho',TM\right] = -0.03511 - 2.29438i \times 10^{-3}$$

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Define functions specific to the ESD-SW calculation.

"Introduction Matrix" P(λ,ρ,κ,t):

- λ - two-element matrix λ=(μ,ν).
- ρ - vector defined as k(**r**-**R**), in spherical coordinates.
- κ - vector specifying direction of incident electron, in spherical coordinates
- t - t-matrix of atom at **R**. t = exp(iδ_l)sin(δ_l) has NL elements.

$$P(\lambda,\rho,\kappa,t) := \left| \begin{array}{l} NL \leftarrow \mathrm{rows}(t) - 1 \\ p \leftarrow \sqrt{4\cdot\pi}\cdot\displaystyle\sum_{l=0}^{NL}\sum_{m=-l}^{l}\Gamma\left[\begin{pmatrix} l \\ m \end{pmatrix},\lambda,\rho\right]\cdot t_l\cdot\overline{Y(l,m,\kappa_1,\kappa_2)} \\ p \end{array} \right.$$

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"Termination Matrix" M(λ,ρ):

λ - two-element matrix λ=(μ,ν).

ρ - vector defined as k(**r**-**R**), in spherical coordinates.

$$M(\lambda,\rho) := \Gamma t\left[\begin{pmatrix} 0 \\ 0 \end{pmatrix},\lambda,\rho\right]$$

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Define plane wave function PW(k,r), k in spherical coordinates, r in cartesian coordinates.

$$PW(sv,r) := \left| \begin{array}{l} K \leftarrow \mathrm{stoc}(sv) \\ \exp(i\cdot K\cdot r) \end{array} \right.$$

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Correct for refraction at the vacuum/solid interface. A more sophisticated treatment would apply different angles for different atomic layers.

The angles θ and φ are the polar and azimuthal angles of incidence in the laboratory reference frame. The κ returned by this function is corrected for the refraction through the inner potential V0.

The magnitude of this vector is k, for all θ and φ.

$$\kappa(\theta,\phi,E,V_0) := \mathrm{ctos}\left[\left[\begin{array}{c} 0.5123\cdot\sqrt{E}\cdot\sin(\theta)\cdot\cos(\phi) \\ 0.5123\cdot\sqrt{E}\cdot\sin(\theta)\cdot\sin(\phi) \\ \sqrt{\left(0.5123\cdot\sqrt{E}\cdot\cos(\theta)\right)^2 - 0.262\cdot V_0}\cdot\dfrac{\cos(\theta)}{|\cos(\theta)|} \end{array}\right]\right]$$

$$\kappa(60\cdot deg, 0\cdot deg, 100, 10) = \begin{pmatrix} 4.86057 \\ 1.15005 \\ \end{pmatrix} \qquad 0.5123\cdot\sqrt{100 - 10} = 4.8601$$

$$\begin{pmatrix} 0 \end{pmatrix} \qquad 60\cdot\deg = 1.0472$$

$$\kappa(120\cdot\deg, 180\cdot\deg, 100, 10) = \begin{pmatrix} 4.86057 \\ 1.99154 \\ 3.14159 \end{pmatrix}$$