Spherical Harmonics

In Rehr and Albers (PRB 41, 8139 (1990)) the spherical harmonics are defined as:

|  |  |  |
| --- | --- | --- |
|  |  |  |

Where

|  |  |  |
| --- | --- | --- |
|  |  |  |

Taken together, then, RA is using Laplace normalized spherical harmonics with the Condon-Shortley phase convention.

|  |  |  |
| --- | --- | --- |
|  |  |  |

For m < 0,

|  |  |  |
| --- | --- | --- |
|  |  |  |

And since

|  |  |  |
| --- | --- | --- |
|  |  |  |
|  |  |  |
|  |  |  |

Giving, finally,

|  |  |  |
| --- | --- | --- |
|  |  |  |

This is really just re-deriving the identity

|  |  |  |
| --- | --- | --- |
|  |  |  |

Rehr notes that since he specializes such that , for m < 0 he can effectively just drop the factor of and replace everywhere.

Now this means that in RA, the Legendre polynomials should *omit* the Condon-Shortley phase, so that instead of the normal definition

|  |  |  |
| --- | --- | --- |
|  |  |  |

Where the are the ordinary Legendre polynomials, we should use

|  |  |  |
| --- | --- | --- |
|  |  |  |

Also, we must be aware that Rehr and Albers use Hartree units and NOT Rydberg units.

Big question is, then, is Messiah using the same convention in his rotation matrices?