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PROOF OF AN ADDITION THEOREM FOR THE SPHERICAL VON NEUMANN FUNCTIONS USING KASTERIN'S FORMULA

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Dealing with modern theory of metals and semiconductors (multiple scattering between so called muffin-tin potentials) the author found recently the following addition theorem[1]

$$i^{\ell} n_{\kappa,L}(\vec{r}_1+\vec{r}_2) = 4\pi \sum_{L_1,L_2} C_{LL_1L_2}\, i^{\ell_1+\ell_2} n_{\kappa,L_1}(\vec{r}_1)\, j_{\kappa,L_2}(\vec{r}_2) \text{ for } r_1 > r_2 . \quad (1)$$

Here the abbreviations

$$j_{\kappa,L}(\vec{r}) \equiv j_{\ell}(\kappa r)\, Y_L(\vec{n}), \quad n_{\kappa,L}(\vec{r}) \equiv n_{\ell}(\kappa r) Y_L(\vec{n}), \quad n \equiv \frac{\vec{r}}{r} \quad (2)$$

are used (in[1] the index κ is dropped for simplicity) with $j_{\ell}(\kappa r)$ and $n_{\ell}(\kappa r)$ as the (regular and singular, respectively) spherical cylinder functions and $Y_L(\vec{n})$ as real linear combinations of the spherical harmonics with the quantum numbers ℓ and m_{ℓ}. The coefficients occuring in (1) are generalized Clebsch-Gordon coefficients

$$C_{LL_1L_2} \equiv \int d\Omega\, Y_L(\vec{n}) Y_{L_1}(\vec{n}) Y_{L_2}(\vec{n}). \quad (3)$$

In the case $\ell = 0$ the relation (1) simplifies to the known formula[2]

$$-\frac{\cos \kappa |\vec{r}_1+\vec{r}_2|}{\kappa |\vec{r}_1+\vec{r}_2|} = 4\pi \sum_L (-1)^{\ell} n_{\kappa,L}(\vec{r}_1)\, j_{\kappa,L}(\vec{r}_2) \quad \text{for } r_1 > r_2 . \quad (4)$$

Vice versa (1) may be considered as generalization of (4). As far as the author knows the corresponding literature, this generalization, in[1] derived by means of complex contour integration, is not published till now.

In the following another simple proof is given using Kasterin's representation of the spherical cylinder functions[3]

$$i^{\ell} j_{\kappa,L}(\vec{r}) = Y_L\left(\frac{\hat{k}}{\kappa}\right)\frac{\sin\kappa r}{\kappa r}, \quad i^{\ell} n_{\kappa,L}(\vec{r}) = Y_L\left(\frac{\hat{k}}{\kappa}\right)(-1)\frac{\cos\kappa r}{\kappa r}, \quad \hat{k} \equiv \frac{\partial}{i\partial \vec{r}}. \tag{5}$$

Really, by means of (4) and Kasterin's formula for the spherical von Neumann functions $n_{\kappa,L}(\vec{r})$ we can write (for $r_1 > r_2$)

$$i^{\ell} n_{\kappa,L}(\vec{r}_1 + \vec{r}_2) = Y_L\left(\frac{\hat{k}_{1,2}}{\kappa}\right) 4\pi \sum_{L_1} i^{\ell_1} n_{\kappa,L_1}(\vec{r}_1)\, i^{\ell_1} j_{\kappa,L_1}(\vec{r}_2). \tag{6}$$

$\hat{k}_{1,2}$ means differentiation with respect to $\vec{r}_1$ or $\vec{r}_2$.

If we differentiate with respect to $\vec{r}_2$, then with Kasterin's formula for the spherical Bessel functions $j_{\kappa,L}(\vec{r})$ with

$$\frac{\sin\kappa r}{\kappa r} = \int \frac{d\Omega'}{4\pi} e^{i\kappa\vec{r}\vec{n}'} \tag{7}$$

and with the completeness of the spherical harmonics $Y_L(\vec{n})$, we obtain (omitting the index 2)

$$Y_L\left(\frac{\hat{k}}{\kappa}\right) i^{\ell_1} j_{\kappa,L_1}(\vec{r}) = \sum_{L_2} C_{LL_1L_2}\, i^{\ell_2} j_{\kappa,L_2}(\vec{r}). \tag{8}$$

Setting (3) into (6), immediately (1) turns out, q.e.d.

Differentiation in (6) with respect to $\vec{r}_1$ yields, of course, the same result. This can be seen by means of the following relation

$$-\frac{\cos \kappa r}{\kappa r} = -\frac{1}{\pi}\int \frac{dk}{\kappa}\,\frac{P}{k^2-\kappa^2}\,k^2\left(\frac{k}{\kappa}\right)^n \frac{\sin kr}{kr}, \tag{9}$$

holding for arbitrary non-negative even numbers n; P means the Cauchy principle value. With (9) and with the fact, that the expansion of $Y_L(\vec{n})$ contains only even (or odd) powers of $\vec{n}$, if ℓ is even (or odd, respectively), we can write Kasterin's formula for the spherical von Neumann functions $n_{\kappa,L}(\vec{r})$ in the following way:

$$i^{\ell}\, n_{\kappa,L}(\vec{r}) = -\frac{1}{\pi}\int \frac{dk}{\kappa}\,\frac{P}{k^2-\kappa^2}\,k^2\left(\frac{k}{\kappa}\right)^{\ell} Y_L\left(\frac{\hat{k}}{k}\right)\frac{\sin kr}{kr}. \tag{10}$$

With (7), (9) and the completeness of the spherical harmonics $Y_L(\vec{n})$ we get from (10)

$$Y_L\left(\frac{\hat{k}}{\kappa}\right) i^{\ell_1} n_{\kappa,L_1}(\vec{r}) = -\frac{1}{\pi}\int \frac{dk}{\kappa}\,\frac{P}{k^2-\kappa^2}\,k^2\left(\frac{k}{\kappa}\right)^{\ell+\ell_1} \sum_{L_2} C_{LL_1L_2}\, Y_{L_2}\left(\frac{\hat{k}}{k}\right)\frac{\sin kr}{kr}. \tag{11}$$

Because $C_{LL_1L_2} = 0$, if $\ell+\ell_1-\ell_2$ is odd or negative, we can replace the exponent $\ell+\ell_1$ by ℓ_2 owing to the independence of (9) from n. Therefore in analogy to (8)

$$Y_L\left(\frac{\hat{k}}{\kappa}\right) i^{\ell_1} n_{\kappa,L_1}(\vec{r}) = \sum_{L_2} C_{LL_1L_2}\; i^{\ell_2} n_{\kappa,L_2}(\vec{r}) \tag{12}$$

turns out. Setting (12) into (6) again (1) follows, q.e.d.

By the way, with (8) and with the known formula[2]

$$\frac{\sin\kappa|\vec r_1+\vec r_2|}{\kappa|\vec r_1+\vec r_2|} = 4\pi\sum_L (-1)^\ell\, j_{\kappa,L}(\vec r_1) j_{\kappa,L}(\vec r_2) \qquad (13)$$

immediately follows the addition theorem for spherical Bessel functions

$$i^\ell j_{\kappa,L}(\vec r_1+\vec r_2) = 4\pi \sum_{L_1,L_2} C_{LL_1L_2}\, i^{\ell_1+\ell_2} j_{\kappa,L_1}(\vec r_1) j_{\kappa,L_2}(\vec r_2), \qquad (14)$$

which has been derived recently by means of the well-known plane-wave expansion formula[4]. The latter vice versa results from (5):

$$4\pi\sum_L i^\ell j_{k,L}(\vec r) Y_L(\vec n') = \int d\Omega'' \sum_L Y_L\left(\frac{\hat k}{k}\right) Y_L(\vec n'') e^{ik\vec r\vec n''} = e^{i\vec k\vec r} \qquad (15)$$

with $\vec k = k\vec n'$.

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R e f e r e n c e s

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