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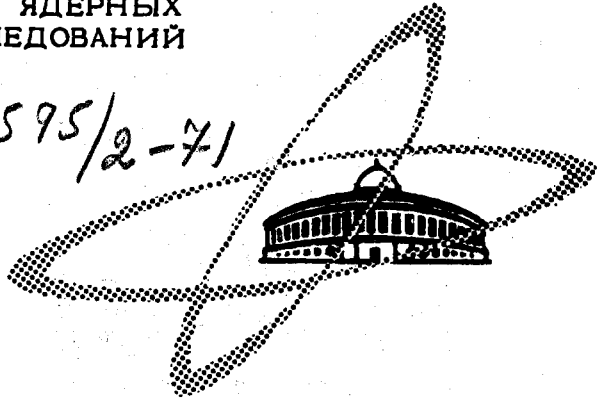
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ЛАБОРАТОРИЯ ТЕОРЕТИЧЕСКОЙ ФИЗИКИ

P.Ziesche

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

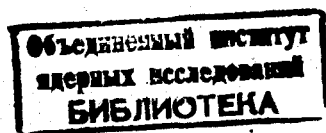
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P.Ziesche *

**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/}

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

Here the abbreviations

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

are used (in^{/1/} the index κ is dropped for simplicity) with $i_{\ell}(\kappa r)$ 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 occurring 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/}

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

Vice versa (1) may be considered as generalization of (4). As far as the author knows the corresponding literature, this generalization, in^{1/1} 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^{1/3/}

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

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

$$i^{\ell} n_{\kappa,L}^{\ell}(\vec{r}_1 + \vec{r}_2) = Y_L\left(\frac{\hat{k}_{1,2}}{\kappa}\right) 4\pi \sum_{L_1} i^{\ell_1} n_{\kappa,L_1}^{\ell_1}(\vec{r}_1) i^{\ell_2} i_{\kappa,L_1}^{\ell_2}(\vec{r}_2). \quad (6)$$

$\hat{k}_{1,2}$ 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 $i_{\kappa,L}^{\ell}(\vec{r})$ with

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

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

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

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

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

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

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:

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

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

$$Y_L\left(\frac{\hat{k}}{\kappa}\right) i^{l_1} n_{\kappa, L_1}(\vec{r}) = -\frac{1}{\pi} \int \frac{dk}{k} \frac{P}{k^2 - \kappa^2} k^2 \left(\frac{k}{\kappa}\right)^{l+l_1} \sum_{L_2} C_{LL_1L_2} Y_{L_2}\left(\frac{\hat{k}}{k}\right) \frac{\sin kr}{kr}. \quad (11)$$

Because $C_{LL_1L_2} = 0$, if $l+l_1-l_2$ is odd or negative, we can replace the exponent $l+l_1$ by l_2 owing to the independence of (9) from n . Therefore in analogy to (8)

$$Y_L\left(\frac{\hat{k}}{\kappa}\right) i^{l_1} n_{\kappa, L_1}(\vec{r}) = \sum_{L_2} C_{LL_1L_2} i^{l_2} n_{\kappa, L_2}(\vec{r}) \quad (12)$$

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

By the way, with (8) and with the known formula^{/2/}

$$\frac{\sin \kappa |\vec{r}_1 + \vec{r}_2|}{\kappa |\vec{r}_1 + \vec{r}_2|} = 4\pi \sum_L (-1)^L i_{\kappa,L}(\vec{r}_1) i_{\kappa,L}(\vec{r}_2) \quad (13)$$

immediately follows the addition theorem for spherical Bessel functions

$$i_{\kappa,L}^{\ell}(\vec{r}_1 + \vec{r}_2) = 4\pi \sum_{L_1, L_2} C_{L, L_1, L_2} i_{\kappa, L_1}^{\ell}(\vec{r}_1) i_{\kappa, L_2}(\vec{r}_2), \quad (14)$$

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

$$4\pi \sum_L i_{\kappa,L}^{\ell}(\vec{r}) Y_L(\vec{n}') = \int d\Omega \sum_L Y_L(\frac{\hat{k}}{k}) Y_L(\vec{n}') e^{i\vec{k}\vec{r}} = e^{i\vec{k}\vec{r}} \quad (15)$$

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

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