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SLOW NEUTRON SCATTERING BY WATER MOLECULES

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C O N T E N T S

LIST OF SYMBOLS

$\sigma(\theta,\varepsilon)$	-	double differential cross section
σ_b	-	boundary value of scattering cross section
E_o	-	energy (in eV) of incoming neutron
E	-	energy (in eV) of scattered incoming neutrons
m	-	mass of molecules
k	-	momentum of scattered neutron
k_o	-	momentum of incoming neutron
κ	-	momentum transfered in collision
$A,B,\bar{E}$	-	Nelkin´s constants
θ	-	angle of scattering
ω	-	energy of molecular vibrations (in eV)
T	-	temperature of medium multiplied by Boltzman´s constant (in eV)
$I_n(x)$	-	modified Bessel function
$\sigma_s(E_o \to E)$	-	scattering kernel
$\sigma_s(E)$	-	scattering cross section
$B_n(x)$	-	Bernoulli polynomial
B_n	-	Bernoulli number
$P_n(t)$	-	polynomial related with Bernoulli polynomials
$F(x,a)$	-	sum
x,θ	-	independent variables
R_{2r}	-	residue
$\hat{A}_{2r},\hat{A},\hat{B},\hat{A}'$	-	operators
Z,P	-	complex numbers
$I(a)$	-	integral
$g(x,a)$	-	relative deviation

$H_\nu(x)$ - Hermitian polynomials

$B(x,a)$ - function (2.4.16)

$\gamma,\delta,\beta_1,\alpha_1$ - defined in (3.10)

α,β - defined in (3.13)

$\tilde{I}_1(\theta_1)$ - function in (3.20)

$M_1(\theta_1), R_1(\theta_1), M(\theta_1)$ - functions

$G_1(E)$, $G_2(E)$ - functions in (5.9), (5.10).

A B S T R A C T

In this work some new, preliminary formulae for slow neutron scattering cross section calculation by heavy and light water molecules have been done. The idea was to find, from the sum which existes in well known Nelkin´s model, other cross sections in more simple analytical form, so that next approximations may be possible. In order to sum a series it was starting from Euler-Maclaurin´s formula. Some new summation formulae have been derived there, and defined in two theorems. A connection between Euler-Maclaurin´s and Poisson´s formulae have also been given as an consequence of derived theorems. Extentive calculations, especially during the evaluation of residues, have been made at the computer CDC 3600. A validity of derived formulae are compared with BNL-325 results, where it is shown a good agreement, as it is well known.

I. INTRODUCTION

Scattering theory of particles becomes last year more and more important in physics and technics. A lot of physical lawfulness can be experimentally determined or checked by scattering of particles. Some new ideas have been emerged from this theory, as for example, dispersion relations, fluctuations and disipations in the system, etc.

Slow neutron scattering theory has also a great importance in physics and technics. In physics it was shown that correlation functions describing the fluctuation and disipation in the system, and giving also the correction of thermodynamical magnitudes in slow neutron scattering theory are related with Fourier transforms of double differential cross section. Neutron physics has also a great application in research of structure and dynamics of the microsystem.

One of terms of the kernel of integral operator in transport equation is the scattering cross section. As it is well known, there are only few types of integral equations that can be analytically solved. This work is a first step in order to obtain such scattering cross section so that it will be possible an analytical solution to the transport equation. It is shown that an expansion to the scattering cross section in degenerate kernel is the most convenient method for formulae given in this work.

Nelkin /1, 2/ found from Zemach-Glauber's work /3/ describing more exactly of the scattering process, a scattering cross section in incoherent approximation:

$$\frac{d^2\sigma}{d\Omega d\epsilon} = \sigma(\theta,\epsilon) = \frac{\sigma_b}{4\pi}\left(\frac{E}{E_o}\right)^{1/2}\left(\frac{m}{2\pi EK^2}\right)^{1/2} \exp\left(-\frac{K^2}{2A}\right) S \qquad (1.1)$$

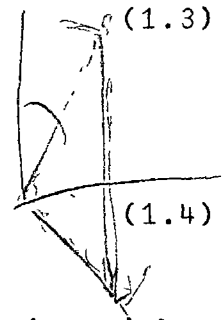
$$S = \sum_{u=-\infty}^{\infty} \exp\left(-\frac{n\omega}{2T}\right) \, \mathrm{In}\left(\frac{K^2}{2B}\right) \exp\left| -\frac{m}{2\bar{E}K^2}\left(E-E_o-n\omega+\frac{K^2}{2m}\right)^2 \right| \qquad (1.2)$$

There is need to find the kernel

$$\sigma_s(E_o \to E) = \int \sigma(\theta,\varepsilon)d\Omega \qquad (1.3)$$

and

$$\sigma_s(E) = \int_0 \sigma(E \to E')dE' \qquad (1.4)$$



Analytical solution to the transport equation with (1.1) is practically impossible and to find $\sigma_s(E_o \to E)$ and $\sigma_s(E)$ also.

It would comment that there are some better models describing a neutron scattering by molecules, but this one is more available.

2. A SERIES SUMMATION

2.1. Bernoulli polynomials and series

A Bernoulli polynomials generating function is

$$\frac{te^{tx}}{e^{t}-1} = \sum_{n=o}^{\infty} \frac{B_n(x)t^n}{n!} \qquad (2.1.1)$$

where $|t| < \alpha < 2\pi$,

α is the convergency radius of the series (2.1.1). It is easily possible to show that $\alpha = 1/2\pi$.

Bernoulli numbers are defined as:

$$B_n(0) \equiv B_n \; , \qquad (2.1.2)$$

or over a generating function

$$\frac{t}{e^{t}-1} = \sum_{n=o}^{\infty} \frac{B_n}{n!} t^n \; , \qquad (2.1.2)$$

with feature characteristics

$$B_o = 1, \quad B_1 = -\frac{1}{2} \; , \quad B_{2n+1} = o, \quad n=1,2,... \qquad (2.1.3)$$

Polynomials

$$P_n(t) \equiv \frac{B_n(t) - B_n}{n!} \qquad (2.1.4)$$

can also be defined, or over the generating function

$$\frac{t(e^{tx}-1)}{e^{x}-1} = \sum_{n=o}^{\infty} P_n(x)t^n \qquad (2.1.5)$$

$$P_{2n}(o) = P_{2n}(1) = 0 \tag{2.1.6}$$

Next formulae are very useful

$$B_{2k}(x) = 2(-1)^{k+1}(2k)! \sum_{r=1}^{\infty} \frac{\cos 2\pi rx}{(2\pi r)^{2k}} \tag{2.1.7}$$

$$B_{2k+1}(x) = 2(-1)^{k+1}(2k+1)! \sum_{r=1}^{\infty} \frac{\sin 2\pi rx}{(2\pi r)^{2k+1}} \tag{2.1.8}$$

$$P_{2k}(x) = (-1)^{k+1}2 \sum_{r=1}^{\infty} \frac{\cos 2\pi rx-1}{(2\pi r)^{2k}} \tag{2.1.9}$$

$$P_{2k+1}(x) = (-1)^{k+1}2 \sum_{r=1}^{\infty} \frac{\sin 2\pi rx-1}{(2\pi r)^{2k+1}} \tag{2.1.10}$$

2.2. Euler-Maclaurin´s formula

Let $f(n+x,a)$ be summable and sufficiently times differentiable function over independent variable x, so that there exists a sum

$$F(x,a) = \sum_{n=-\infty}^{\infty} f(n+x,a) \ , \tag{2.2.1}$$

where are

x - independent variable

with the help of a we denote an array of constants $a_1,\dots,a_2$, then Euler-Maclaurin´s formula

$$\sum_{n=-\infty}^{\infty} f(n+x,a) = \int_{-\infty}^{\infty} f(y+x,a)dy + \lim_{y\to\infty} \Big\{ f(y+x,a) + f(-y+x,a) + \sum_{k=1}^{\infty} \frac{B_k}{k!}\Big[f^{(k-1)}_{(y+x,a)} - f^{(k-1)}_{(-y+x,a)}\Big]\Big\} + R \tag{2.2.2}$$

written in the case of infinite limits, is valid /4/.

We will always denote $f^{(\nu)}_{(y+x,a)}$ as ν-th derivation over y-variable.

R is the residue:

$$R = \lim_{r\to\infty} R_{2r} = \lim_{r\to\infty} \int_0^1 dt\ P_{2r+2}(t) \sum_{k=-\infty}^{\infty} f^{(2r+2)}_{(t+x+k,a)} \qquad (2.2.3)$$

2.3. Some summation formulae

Now we will show some very useful formulae, that can be find from expression (2.2.2) for a special class of functions.

Let be

$$\lim_{y\to\pm\infty} f^{(k-1)}_{(y+x,a)} = o \ , \quad \text{for} \quad k=1,2,\dots, \qquad (2.3.1)$$

then next lemma is valid:

Lemma 1.

$$\lim_{y\to\pm\infty} \sum_{k=1}^{\infty} \frac{B_k}{k!} f^{(k-1)}_{(y+x,a)} = o \qquad (2.3.2)$$

for finite x.

This lemma is obvious as we remark that

$$\lim_{k\to\infty} \left| \frac{B_k}{n!} \right| = o \ , \quad \text{and conditions (2.3.1)}$$

Let us introduce now following denotations

$$F(x,a) = \sum_{n=-\infty}^{+\infty} f(n+x,a) \qquad (2.3.3)$$

$$I(a) = \int_{-\infty}^{\infty} f(y+x,a)dy \qquad (2.3.4)$$

Theorem 1. If function $f(n+x,a)$ satisfies conditions (2.3.1), then expression (2.2.2) can be written in the form

$$F(x,a) = I(a) + \hat{A}F(t+x,a) \ , \qquad (2.3.5)$$

where $\hat{A}$ is an operator over variable t.

Proof: With the help of (2.3.2) we can expression (2.2.2) writte in the form

$$\sum_{n=-\infty}^{\infty} f(n+x,a) = \int_{-\infty}^{\infty} f(y+x,a)dy + \lim_{r\to\infty} R_{2r} \qquad (2.3.6)$$

$$R_{2r} = \int_0^1 dt\ R_{2r+2}(t) \sum_{k=-\infty}^{+\infty} f^{(2r+2)}_{(t+k)}$$

$$= \sum_{k=-\infty}^{+\infty} \int_0^1 dt\ R_{2r+2}(t) \frac{(2r+2)!}{2\pi i} \oint_{\Gamma_1} \frac{f(z+x,a)dz}{z-(t+x)^{2r+3}}$$

$$= \sum_{k=-\infty}^{\infty} \int_0 dt\ P_{2r+2}(t) \frac{(2r+2)!}{2\ i} \oint_{\Gamma_2} \frac{f(z+t+x+k,a)dz}{z^{2r+3}} \qquad (2.3.7)$$

where are Γ_1: $|z-(t+k)| < 1$ and Γ_2: $|z| < 1$.

Expression (2.3.7) may be transformed in the form

$$R_{2r} = \int_0^1 dt\ P_{2r+2}(t) \frac{(2r+2)!}{2\pi i} \oint_{\Gamma_2} \frac{\sum_{k=-\infty}^{\infty} f(k+z+t+x,a)}{z^{2r+3}} dz$$

$$= \int_0^1 dt\ P_{2r+2}(t) \frac{(2r+2)!}{2\pi i} \oint_{\Gamma_2} \frac{\Gamma(z+t+x,a)dz}{z^{2r+3}}$$

$$= \int_0^1 dt\ P_{2r+2}(t) \frac{d^{2r+2}F(t+x,a)}{dt^{2r+2}} \qquad (2.3.8)$$

So we proved that

$$R_{2r} = \hat{A}_{2r}F(t+x,a) \qquad (2.3.8)$$

$$\hat{A}_{2r} = \int_0^1 dt\ P_{2r+2}(t)\frac{d^{2r+2}}{dt^{2r+2}}\ (\cdot) \qquad (2.3.9)$$

$$\lim_{r\to\infty} \hat{A}_{2r} = \hat{A} \qquad (2.3.10)$$

With the help of (2.3.9), (2.3.6) and using the denotations (2.3.3) and (2.3.4) we can writte

$$F(x,a) = I(a) + \hat{A}F(x+t,a) \qquad (2.3.11)$$

So theorem 1 is proved.

As I(a) does not depend of x, then defining a new variable

$$g(x,a) \equiv (F(x,a) - I(a))/I(a) \quad , \qquad (2.3.12)$$

expression (2.3.11) may be written in the form

$$g(x,a) = \hat{A}g(x+t,a) \qquad (2.3.13)$$

Function $g(x,a)$ has a sense as relative deviation of the sum from the integral.

2.4. A connection between Euler-Maclaurin's and Poisson's formula

It is possible to show that

$$F(x,a) = F(-x,a)$$

$$g(x,a) = g(-x,a) \ , \qquad (2.4.1)$$

then we can writte the equation (2.3.13) in the form

$$g(x,a)\ \hat{A}^{*}_{2r}g(x+t,a) \qquad (2.4.2)$$

$$\hat{A}'_{2r} = \frac{1}{2} \int_{-1}^{+1} dt \; P_{2r+2}(t) \; \frac{d^{2r+2}(\cdot)}{dt^{2r+2}} \tag{2.4.3}$$

Theorem 2. The solution of the equation (2.4.2) has the form

$$g(x,a) = \sum_{k=1}^{\infty} A_k(a) \cos(2\pi kx) \; , \tag{2.4.4}$$

where $A_k(a)$ are some unknown functions that depend only of a.

Proof: Using $P_{2r+2}(t)$ from (2.1.9) and representing together with (2.4.4) in (2.4.2) we have

$$g(x,a) = \sum_{k=1}^{\infty} \sum_{j=1}^{\infty} \left(\frac{j}{k}\right)^{2r+2} A_j(a) \int_{-1}^{1} (\cos 2\pi kt - 1) \cos [2\pi j(t+x)] dt . \tag{2.4.5}$$

As

$$\int_{-1}^{+1} (\cos 2\pi kt - 1) \cos [2\pi j(t+x)] dt = \delta_{nk} \cos(2\pi jx) \; , \tag{2.4.6}$$

(2.4.5) reduces to

$$g(x,a) = \sum_{k=1}^{\infty} \sum_{j=1}^{\infty} \left(\frac{j}{k}\right)^{2r+2} A_j(a) \cos(2\pi jx) \delta_{jk}$$

$$= \sum_{k=1}^{\infty} A_k(a) \cos(2\pi kx) \; . \tag{2.4.7}$$

So we proved the theorem 2.

Functions $A_k(a)$ can be determined from (2.4.4):

$$A_k(a) = \int_{-1}^{1} g(x,a) \cos(2\pi kx) dx$$

$$= \int_{-1}^{1} g(x,a) e^{-2\pi ikx} dx \; . \tag{2.4.8}$$

As

$$F(x,a) = I(a)\left[1 + \sum_{k=1}^{\infty} A_k(a)\cos(2\pi kx)\right] , \qquad (2.4.9)$$

we have

$$A_k(a) = I(a)^{-1} \int_{-1}^{1} F(x,a)e^{-2\pi ikx}dx$$

$$= I^{-1}(a) \sum_{n=-\infty}^{\infty} \int_{-1}^{1} f(x+n,a)e^{-2\pi ikx}dx$$

$$= I^{-1}(a) \sum_{n=-\infty}^{\infty} \int_{n-1}^{n+1} f(x,a)e^{-2\pi ikx}\,dx$$

$$= 2I^{-1}(a) \int_{-\infty}^{\infty} f(x,a)e^{-2\pi ikx}\,dx \qquad (2.4.10)$$

Puting (2.4.10) into (2.4.8) we have

$$\sum_{n=-\infty}^{\infty} f(n+x,a) = 2 \sum_{k=o}^{\infty} \cos(2\pi kx) \int_{-\infty}^{\infty} f(t,a)e^{-2\pi ikt}\,dt ,$$

or in the other form

$$\sum_{n=-\infty}^{\infty} f(n+x,a) = \sum_{n=-\infty}^{\infty} \int_{-\infty}^{\infty} f(t+x,a)e^{-2\pi int}\,dt \qquad (2.4.11)$$

Expression (2.4.11) is well known Poisson´s formula. So we proved that in a special case, when limits of summation are infinite and $f(n+x,a)$ satisfies conditions (2.3.1), Euler-Maclaurin´s formula reduces to the Poisson´s. Surely, Euler-Maclaurin´s formula is more general and gives us a lot of possibility of applications.

In the case of finite limits, an expression similar as (2.3.5) may be done

$$F(x,a) = I(x,a) + \hat{A}F(t+x,a) + B(x,a) \qquad (2.4.12)$$

$$F(x,a) = \sum_{k=m}^{n} f(k+x,a) \qquad (2.4.13)$$

$$I(x,a) = \int_{m}^{n} f(t+x,a)dt \qquad (2.4.14)$$

$$\hat{A} = \lim_{r\to\infty} \int_{0}^{1} dt' P_{2r+2}(t) \frac{d^{2r+2}}{dt^{2r+2}} (\cdot) \qquad (2.4.15)$$

$$B(x,a) = f(m+x,a) + f(n+x,a) + \sum_{k=1}^{\infty} \frac{B_k}{k!} f^{(k-1)}(y+x,a) \Big|_{y=m}^{y=n}$$

$$\ldots\ldots \qquad (2.4.16)$$

2.5. Summation of the series $\sum_{-\infty}^{\infty} \exp(-an^2+2bn)$

Formula (2.3.13) is very useful for approximate summation of series if the solution of summation has again form of any series, but which converges faster the first one.

Let us denote now

$$F(b,a) = \sum_{n=-\infty}^{\infty} \exp(-an^2+2bn) , \qquad a > o \qquad (2.5.1)$$

$$I(b,a) = \int_{-\infty}^{+\infty} \exp(-an^2+2bn)dn = \sqrt{\frac{\pi}{a}}\, e^{\frac{b^2}{a}} \qquad (2.5.2)$$

We can here apply the same method as during the evaluation (2.3.11) and (2.3.13).

Let be

$$f(n,a,b) = \exp(-an^2 + 2bn) , \qquad (2.5.3)$$

and

$$\frac{d^\nu f(x,a,b)}{dx^\nu} = (-1)^\nu a^{\nu/2} f(x,a,b) H_\nu(\sqrt{a}x - \frac{b}{\sqrt{a}}) \qquad (2.5.4)$$

where $H\,(\sqrt{a}x - \frac{b}{\sqrt{a}})$ is the Hermitian polynomial:

$$H_\nu(\sqrt{a}x - \frac{b}{\sqrt{a}}) = \frac{\nu!}{2\pi i} \oint_\Gamma \frac{e^{-s^2+2s(\sqrt{a}x - \frac{b}{\sqrt{a}})}}{s^{\nu+1}}\, ds \qquad (2.5.5)$$

Γ: $|s| < 1$.

It is easily to show that

$$R_{2r} = \hat{R}_{2r}F(a,b_1)$$
$$b_1 = b - at + s\sqrt{a} \qquad (2.5.6)$$

$$\hat{R}_{2r} = s^{r+1}\int_0^1 dt\, P_{2r+2}(t)f(t,a,b)\, \frac{(2r+2)!}{2\pi i} \oint_\Gamma \frac{e^{-s^2+2[\sqrt{a}t - \frac{b}{\sqrt{a}}]\, s}}{s^{2r+3}}\, ds(\cdot) \quad \ldots\ldots \qquad (2.5.7)$$

If we represent $F(a,b)$ in the form

$$F(a,b) = I(a,b)g(a,b)\ , \qquad (2.5.8)$$

where $g(a,b)$ is an unkown function, and $I(a,b)$ defined in (2.5.2), then follows

$$\hat{R}_{2r}\Big[I(a,b_1)g(a,b_1)\Big] = I(a,b)\hat{B}_{2r}g(a,b_2) \qquad (2.5.9)$$

$$\hat{B}_{2r} \equiv a^{2r+2}\int_0^1 dt\, P_{2r+2}(t)\, \frac{d^{2r+2}(\cdot)}{db_2^{2r+2}} \qquad (2.5.10)$$

$$b_2 = b - at$$

It is possible to show

$$\hat{R}_{2r}I(a,b_2) = o\ . \qquad (2.5.11)$$

With the help of (2.5.11) and (2.5.9) we have

$$g(a,b) = \hat{B}g(a,b_2) \qquad (2.5.12)$$

$$g(a,b) \equiv (F(a,b) - I(a,b))/I(a,b) \qquad (2.5.13)$$

The solution of the equation (2.5.12) can be written as

$$g(a,b) = \sum_{k=1}^{\infty} A_k(a)\cos\left(\frac{2\pi bk}{a}\right) , \qquad (2.5.14)$$

if we used (2.1.9) expansion for $P_{2r+2}(t)$ with a condition

$$g(a,b) = g(a,-b) \qquad (2.5.15)$$

The simplest method to find unknown coefficients $A_k(a)$ is a Poisson´s formula

$$\sum_{k=-\infty}^{\infty} f(2\pi k) = \frac{1}{2\pi} \sum_{k=-\infty}^{\infty} \int_{-\infty}^{\infty} f(\tau)e^{-ik\tau}d\tau , \qquad (2.5.16)$$

from where we find

$$A_k(a) = 2e^{-\frac{\pi^2 k^2}{a}} \qquad (2.5.17)$$

From (2.5.16) follows that it is possible to derive the expression (2.5.14) without Euler-Maclaurin´s formula, but Euler-Maclaurin´s formula is more general then Poisson´s especially because the residue need not be expanded in a series. Here the form (2.5.14) is very convenient, because function $g(a,b)$ is bounded over a and b, and coefficients converge more faster so that it is possible to take only few first terms.

Finally, we can writte

$$\sum_{n=-\infty}^{+\infty} e^{-an^2+2bn} = \sqrt{\frac{\pi}{a}}\, e^{\frac{b^2}{a}} (1+g(b,a)) , \qquad (2.5.18)$$

$$o \le |g(a,b)| \le 2$$

for $o \le a < \infty$, and

$-\infty < b < \infty.$

3. SCATTERING LAW

We start from the expression (1.1)

$$\sigma(\theta,\varepsilon) = \frac{\sigma_b}{4r} \left(\frac{E}{E_o}\right)^{1/2} \left(\frac{m}{2\pi\bar{E}k^2}\right)^{1/2} \exp\left(-\frac{K^2}{2A}\right) S \tag{3.1}$$

where

$$S = \sum_{n=-\infty}^{\infty} \exp\left(-\frac{n\omega}{2T}\right) I_n\left(\frac{K^2}{2B}\right) \exp\left[-\frac{m}{2\bar{E}k^2}\left(E-E_o-n+\frac{K^2}{2m}\right)^2\right] \tag{3.2}$$

$\vec{K} = \vec{k} - \vec{k}_o$ - momentum transfered,

$-\varepsilon = E - E_o$ - energy transfered,

$m, \bar{E}, A, B$ - are given positive constants, that depend only in particular energy intervals of incoming neutrons.

If we writte the Bessel function I_n as the integral

$$I_n(x) = \frac{1}{\pi}\int_0^{\pi} e^{\beta_1 \cos\theta_1} \cos n\theta_1 d\theta_1 , \tag{3.3}$$

the sum (3.2) can be written in the form

$$I(\theta_1) = \sum_{n=-\infty}^{\infty} \exp\left[-n\alpha_1-\gamma(\delta-n\omega)^2\right]\cos n\theta_1 \tag{3.5}$$

Instead of $I(\theta_1)$ we may consider

$$\tilde{I}(\theta_1) = \sum_{n=-\infty}^{\infty} \exp\left[-n\alpha_1-\gamma(\delta-n\omega)^2-ni\theta_1\right] , \tag{3.6}$$

so that $I(\theta_1) = \mathrm{Re}\,\{\tilde{I}(\theta_1)\}$, and

$$\tilde{I}(\theta_1) = \sum_{n=-\infty}^{\infty} \tilde{A}_n(\theta_1) \tag{3.7}$$

$$\tilde{A}_n(\theta_1) = \sqrt{\frac{\pi}{\gamma\omega 2}} \exp(Q_n(\theta_1)) \tag{3.8}$$

$$Q_n(\theta_1) = \frac{P(P-4\omega\delta\gamma)}{4\gamma\omega^2} + \frac{2\pi i(\gamma\delta\omega - P/2)}{\gamma\omega^2} n - \frac{\pi^2 n^2}{\gamma\omega^2} \tag{3.9}$$

$P = \alpha_1 + i\theta_1$,

where these signs are used

$$\gamma = \frac{m}{2\bar{E}k^2}, \quad \frac{K^2}{2m} - \varepsilon = \delta, \quad \frac{K^2}{2B} = \beta_1, \quad \alpha_1 = \frac{\omega}{2T} \tag{3.10}$$

With the help of derived expressions we can finally writte

$$\sigma(\theta,\varepsilon) = \frac{\sigma_b}{4\pi\omega} \left(\frac{E}{E_o}\right)^{1/2} \exp\left(-\frac{K^2}{2A}\right) \frac{1}{\pi} \int_o^{\pi} \sum_{n=-\infty}^{\infty} \exp(\beta_1 \cos\theta_1\ Q_n(\theta_1)) d\theta_1 \quad \ldots\ldots \tag{3.11}$$

The double differential scattering cross section can be written in the form:

$$\tau(\theta, \ ) = \frac{\tau_b}{4T} \left(\frac{E}{E_o}\right)^{1/2} e^{-\beta/2} S(\alpha,\beta) \tag{3.12}$$

$$\left.\begin{aligned} \alpha &= \frac{E+E_o-2(EE_o)^{1/2}\cos\theta}{mT} = \frac{K^2}{2mT} \\ \beta &= \frac{E - E_o}{T} \end{aligned}\right\} \tag{3.13}$$

Next connection is available

$$\gamma = \frac{1}{4\bar{E}T\alpha}, \quad \delta = T(\alpha+\beta), \quad \beta_1 = \frac{mT\alpha}{B} \tag{3.14}$$

Comparing (3.12) and (3.11) we can find

$$S(\alpha,\beta) = \frac{T}{\pi\omega} \exp\left(\frac{\beta}{2} - \frac{mT\alpha}{2}\right) \frac{1}{\pi} \sum_{n=-\infty}^{\infty} \int_o^{\pi} \exp(\beta, \cos\theta_1 + Q_n(\theta_1)) d\theta_1 \tag{3.15}$$

But, there is one else possibility to express the scattering cross section. Namely, sum (3.6) is in the other form

$$\tilde{I}(\theta_1) = \sqrt{\frac{\pi}{a}} \sum_{n=-\infty}^{\infty} e^{\frac{(b-n\pi)^2}{a}} \qquad (3.16)$$

$a = \gamma\omega^2$, $\quad b = \gamma\delta\omega - P/2$, $\quad P = \alpha_1 + i\theta_1$

$$b - in\pi = \gamma\delta\omega - \frac{\alpha_1 + i(\theta_1 + 2n\pi)}{2} ,$$

and expression (3.4) reduces to

$$S = \sum_{n=-\infty}^{\infty} \frac{1}{\pi} \int_0^{\pi} \exp\left\{\beta_1 \cos\theta_1 - \gamma\omega^2 + \frac{[\gamma\delta\omega - \alpha_1 - i(\theta_1 + 2n\pi)]^2}{4\gamma\omega^2}\right\} d\theta_1$$

$$= \sum_{n=-\infty}^{\infty} \frac{1}{\pi} \int_{2n\pi}^{(2n+1)\pi} \exp\left\{\beta_1 \cos\theta_1 - \gamma\omega^2 + \frac{(\gamma\delta\omega - P/2)^2}{\gamma\omega^2}\right\} d\theta_1$$

$$= \frac{1}{\pi} \int_{-\infty}^{\infty} \exp\left\{\beta_1 \cos\theta_1 - \gamma\omega^2 + \frac{(\gamma\delta\omega - P/2)^2}{\gamma\omega^2}\right\} d\theta_1 \qquad (3.17)$$

Finally

$$\sigma(\theta,\varepsilon) = \frac{\sigma_b}{4\pi\omega}\left(\frac{E}{E_o}\right)^{1/2} \exp\left(-\frac{K^2}{2A}\right) \frac{1}{\pi} \int_{-\infty}^{\infty} e^{\beta_1 \cos\theta_1} \tilde{I}_1(\theta_1) d\theta_1 \qquad (3.18)$$

and

$$S(\alpha,\beta) = \frac{T}{\pi\omega} \exp\left(\frac{\beta}{2} - \frac{mT}{A}\alpha\right) \frac{1}{\pi} \int_{-\infty}^{\infty} e^{\beta_1 \cos\theta_1} \tilde{I}_1(\theta_1) d\theta_1 \qquad (3.19)$$

$$\tilde{I}_1(\theta_1) = \exp\left(\frac{P(P - 4\omega\delta\gamma)}{4\gamma\omega^2} \right) \qquad (3.20)$$

4. $\sigma(E_o \rightarrow E)$ DERIVATION

The kernel $\sigma(E_o\rightarrow E)$ is

$$\sigma(E_o\rightarrow E) = \int_\Omega \sigma(\theta,\varepsilon)d\Omega = \frac{\pi}{kk_o}\int_{(k-k_o)^2}^{(k+k_o)^2} \sigma(\theta,\varepsilon)dk^2 \qquad (4.1)$$

Cross section $(\theta, \ )$ from (3.18) in other form

$$\sigma(\theta,\varepsilon) = \frac{\sigma_b}{4\pi\omega}\left(\frac{E}{E_o}\right)^{1/2}\frac{2}{\pi}\int_{-\infty}^{\infty} e^{k^2M(\theta_1)+R_1(\theta_1)}d\theta_1 \qquad (4.2)$$

$$M_1(\theta_1) = \frac{P(P\frac{\bar{E}}{\omega} - 1)}{2m\omega}$$

$$P = \alpha_1 + i\theta_1 , \qquad R_1 = P\frac{\varepsilon}{\omega} ,$$

$$M(\theta_1) = -\frac{1}{2A} + \frac{1}{2B}\cos\theta_1 + M_1(\theta_1)$$

After integration in (4.1) we get

$$\sigma(E_o\rightarrow E) = \frac{\sigma_b}{4\pi\omega k_o^2}\int_{-\infty}^{\infty} e^{R_1(\theta_1)}\frac{e^{(k+k_o)^2M} - e^{(k-k_o)^2M}}{M}d\theta_1 \qquad (4.3)$$

From (4.3) it is very easily to **take** the sum as in expression (3.17).

5. $\sigma_s(E)$ DERIVATION

Cross section $\sigma_s(E)$ is defined as

$$\sigma_s(E) = \int_0^\infty \sigma(E\to E')dE' = \int_0^\infty \sigma(E\to E')k'dk' \qquad (5.1)$$

Integrating the kernel $\sigma(E\to E')$ from (4.3) we get immediately

$$\sigma_s(E) = \frac{\sigma_b}{2}\sqrt{\frac{\omega}{\pi E}}\int_{-\infty}^{\infty}\frac{\exp\left[\frac{E\ P^2}{\omega(P-2\omega M)}\right]}{(P-2\omega M)^{3/2}}\,d\theta_1 \qquad (5.2)$$

for $E\ \varepsilon(0,15;\ 0,2)$ eV.

In region $0,15\ \text{eV} < E < 0,2\ \text{eV}$ constants A, B, m, ω and $\bar{E}$ depend if the energy transfered is less or greater than 0,01 eV, namely $|E\to E_o| \lessgtr 0,01\ \text{eV} = \Delta$.

Let us denote with sign 1 all constants that can be find with constants for $|E\to E_o| > \Delta$, and with sign 2 constants for which $|E\to E_o| < \Delta$.

According to (5.1) in region $0,15 < E < 0,2$ we have

$$\sigma_s(E_o) = \int_0^{E_o-\Delta}\sigma_1(E_o,E)dE + \int_{E_o-\Delta}^{E_o+\Delta}\sigma_2(E_o,E)dE + \int_{E_o+}^{\infty}\sigma_1(E_o,E)dE \qquad (5.3)$$

As Δ is very small, then in (5.3) we may expend to a series over Δ powers.

$$\int_0^{E_o-\Delta}\sigma_1(E_o,E)dE = \int_0^{E_o}\sigma_1(E_o,E)dE - \Delta\sigma_1(E_o,E_o) + \frac{\Delta^3}{6}\left.\frac{\partial^2\sigma_1(E_o,x)}{\partial x^2}\right|_{x=E_o} + \dots$$

$$\dots\dots \qquad (5.4)$$

where we used the condition

$$\left.\frac{\partial\sigma(E_o,x)}{\partial x}\right|_{E_o=x} = 0 \qquad (5.5)$$

We can also find

$$\int_{E_o-\Delta}^{E_o+\Delta}\sigma_2(E_o,E)dE = 2\Delta\sigma_2(E_o,E_o) + \frac{\Delta^3}{3}\left.\frac{\partial^2\sigma_2(E_o,x)}{\partial x^2}\right|_{x=E_o} + \ldots \qquad (5.6)$$

and

$$\int_{E_o+\Delta}^{\infty}\sigma_1(E_o,E)dE = \int_{E_o}^{\infty}\sigma_1(E_o,E)dE - \Delta\sigma_1(E_o,E_o) - $$

$$- \frac{\Delta^3}{6}\left.\frac{\partial^2\sigma_1(E_o,x)}{\partial x^2}\right|_{x=E_o} + \ldots \qquad (5.7)$$

Representing (5.7), (5.8) and (5.4) in (5.3) we get

$$\sigma_s(E) = \sigma_1(E) + \Delta G_1(E) + \Delta^3 G_2(E) \qquad (5.8)$$

$$G_1(E) = 2\left[\sigma_2(E,E) - \sigma_1(F,E)\right] \qquad (5.9)$$

$$G_2(E) = \frac{1}{3}\left.\frac{\partial^2\sigma_2(E_o,x)}{\partial x^2}\right|_{x=E_o} \qquad (5.10)$$

E - is the energy of incoming neutron.

A similar expression for scattering cross section as sum can also be find on the same method as earlier.

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