AN APPROXIMATE METHOD FOR SOLVING THE INTEGRAL EQUATION OF TRANSPORT THEORY

M. I. Zhurina, A. M. Popova, and A. P. Prudnikov

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An approximate solution is given for one of the integral equations of transport theory, using the Pade method.

To determine the probability for scattering of particles in a spherically symmetric potential g·V(r) we have the integral equation [1]

$$t(\mathbf{p},\mathbf{p}',k^2)=gV(\mathbf{p},\mathbf{p}')+\int\limits_{\Omega_1}\frac{g\cdot V(\mathbf{p},\mathbf{p}'')\cdot t(\mathbf{p}'',\mathbf{p}',k^2)}{k^2-(p'')^2+i\varepsilon}d\mathbf{p}'', \tag{1}$$

where

$$g\cdot V(\mathbf{p},\mathbf{p}')=\frac{1}{(2\pi)^3}\int\limits_{\Omega_2}\exp\left[-i(\mathbf{p}-\mathbf{p}')\mathbf{r}\right]\cdot g\cdot V(\mathbf{r})\,d\mathbf{r}. \tag{2}$$

Here the factor g in front of the potential function is a numerical parameter $g \le 1$ determining the force of interaction of the particle with the field.

It is known that for all real p and p' the function $t(\mathbf{p},\mathbf{p}',k^2)$ can be expanded in Legendre polynomials

$$t(\mathbf{p},\mathbf{p}',k^2)=\frac{1}{4\pi}\sum_{l=0}^{\infty}(2l+1)\cdot t_l(p,p',k^2)\cdot P_l(\cos\vartheta), \tag{3}$$

where

$$\cos(\vartheta)=(\mathbf{n},\mathbf{n}_1);\quad \mathbf{n}=\frac{\mathbf{p}}{p};\quad \mathbf{n}_1=\frac{\mathbf{p}'}{p'}.$$

Since the function $V(\mathbf{p},\mathbf{p}')$ can also be expanded in Legendre polynomials, then the function $t_l(p,p',k^2)$ is a partial amplitude and satisfies the equation

$$t_l(p,p',k^2)=g\cdot V_l(p,p')+\frac{2}{\pi}\int\limits_0^{\infty}\frac{g\cdot V_l(p,p'')\cdot t_l(p'',p',k^2)(p'')^2}{k^2-(p'')^2+i\varepsilon}dp''. \tag{4}$$

where p, p', and k^2 are positive real quantities;

$$g\cdot V_l(p,p')=\int\limits_0^{\infty}j_l(p\cdot r)\cdot g\cdot V(r)\cdot j_l(p'\cdot r)\,r^2dr, \tag{5}$$

$j_l(y)=\sqrt{(\pi/2y)}\,J_{l+1/2}(y)$ are spherical Bessel functions; $J_{l+1/2}(y)$ are cylindrical Bessel functions; and g·V(r) is some real function.

The iteration series in Eq. (4) has a definite physical meaning, and its terms are contributions of n-fold (n = 1, 2, 3, ...) scattering of an incident particle at the given potential. Therefore, to solve a number of scattering problems it is interesting to find the partial probability amplitude $t_l(p,p',k^2)$ using Eq. (4) and the method of successive approximations. However, the iterative series of Eq. (4) converges slowly for positive real values k^2.

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We can accelerate the convergence of the series of successive approximations in solving Eq. (4) by making the assumption that the interaction potential $V_l(p, p')$ is a function of the parameter g:

$$V_l(p, p') = g \cdot V_l'(p, p'). \tag{6}$$

In this case the function $t_l(p, p', k^2)$ becomes independent of the parameter g and we can represent the iteration series of Eq. (4) in the form

$$t_l(p, p', k^2; g) = g \cdot V_l'(p, p') + g^2 \cdot \left(\frac{2}{\pi}\right) \int_0^\infty \frac{V_l'(p, p'') \cdot V_l'(p'', p') \cdot (p'')^2 dp''}{k^2 - (p'')^2 + i\varepsilon}$$

$$+ g^3 \left(\frac{2}{\pi}\right)^2 \int_0^\infty \int_0^\infty \frac{V_l'(p, p'') \cdot V_l'(p'', p''') \cdot V_l'(p''', p')(p'')^2 \cdot (p''')^2 \cdot dp'' \cdot dp'''}{(k^2 - (p'')^2 + i\varepsilon) \cdot (k^2 - (p''')^2 + i\varepsilon)} + \dots \tag{7}$$

Since the series (7) converges slowly for g = 1 and large k^2, it is expedient in practice to adjust the Pade method to a different rapidly convergent series. The essence of the Pade method is that the desired function $t_l(p, p', k^2; g)$ is represented as a ratio of two polynomials of degrees n and m:

$$t_l(p, p', k^2; g) = \frac{P_n(g)}{Q_m(g)} + O(g^{n+m+1}). \tag{8}$$

It was shown in [2] that to solve an equation of Fredholm type we can obtain a better approximation for the desired function by using the diagonal Pade approximation

$$t_l(p, p', k^2; g) = \frac{\sum_{\alpha=0}^{n} a_\alpha g^\alpha}{\sum_{\beta=0}^{n} b_\beta g^\beta} + O(g^{2n+1}) \tag{9}$$

and setting $b_0 = 1$. The function $t_l(p, p', k^2; g)$ is analytic in g in a circle of radius $|\rho| \le 1$. Let the series $\sum_{\beta=0}^{n} b_\beta g^\beta$ converge in the circle of the same radius ρ; then we have the relation

$$\frac{\sum_{\alpha=0}^{n} a_\alpha g^\alpha}{\sum_{\beta=0}^{n} b_\beta g^\beta} = c_1 + g \cdot c_2 + g^2 \cdot c_3 + \dots \tag{10}$$

to an accuracy including terms of order $O(g^{2n+1})$. Here the right side is a symbolic representation of the iteration series (7). From Eq. (10), by equating coefficients for the same powers of g on the right and left sides, we can obtain a system of algebraic equations to determine the coefficients a_α and b_β in Eq. (9):

$$\begin{aligned} a_0 &= b_0 \cdot c_1, \\ a_1 &= b_1 \cdot c_1 + b_0 \cdot c_2, \\ a_2 &= b_2 \cdot c_1 + b_1 \cdot c_2 + b_0 \cdot c_3, \\ a_3 &= b_3 \cdot c_1 + b_2 \cdot c_2 + b_1 \cdot c_3 + b_0 \cdot c_4. \\ &\dots\dots\dots\dots \end{aligned} \tag{11}$$

Clearly, any approximation in Eq. (9) is an n-term fraction. It is known from the theory of infinite continued fractions that odd values of n give better approximations [3]. It follows from Eq. (11) that we can find an expression for $t_l(p, p', k^2; g)$ in the linear and cubic Pade approximations of the form [4]

$$t_l^{\text{lin}}(p, p', k^2; g) = \frac{c_1 + g \cdot (c_2 - c_1 \cdot c_3/c_2)}{1 - g(c_3/c_2)}, \tag{12}$$

$$t_l^{\text{cub}}(p, p', k^2; g) = \frac{c_1 + g(c_2 + D_1 \cdot c_1/D) + g^2 \cdot (c_3 + D_1 \cdot c_2/D + D_2 \cdot c_1/D) + g^3 \cdot (c_4 + D_1 \cdot c_3/D + D_2 \cdot c_2/D + D_3 \cdot c_1/D)}{(1 + g \cdot D_1/D + g^2 \cdot D_2/D + g^3 \cdot D_3/D)}, \tag{13}$$

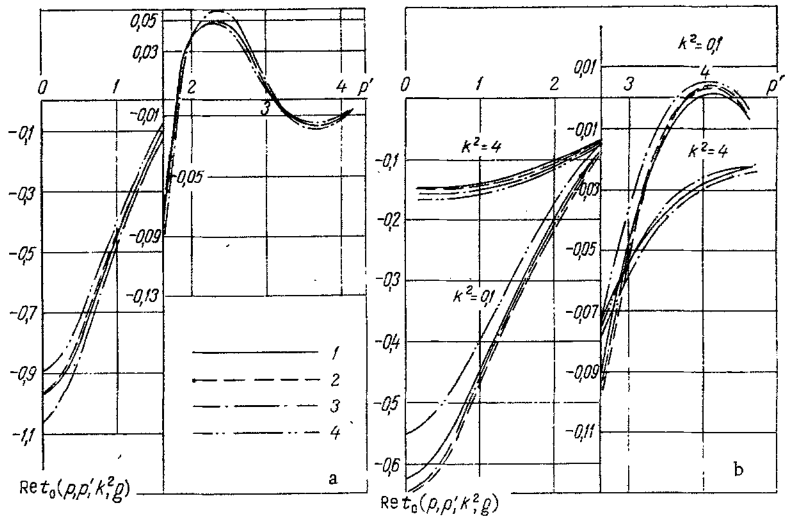

Fig. 1. Real part of the solution of the integral equation for the case of a Woods—Saxon potential a ($V_0 = 0.36\ m^{-2}$, $r_0 = 2.46$ m, $a =$ 0.2 m, $k^2 = 0.1\ m^{-2}$) and a Gauss potential b ($V_0 = 1.9\ m^{-2}$, $r_0 = 1.1$ m, $a = 0.2$ m, $k^2 = 0.1$ and 4 m^{-2}), determined by the method of successive approximations: curve 1) linear approximation; 2) fourth- and higher-order approximations; 3) linear approximation; 4) cubic approximation and an approximation determined by the method described in this paper.

where

$$D = \begin{vmatrix} c_4 & c_3 & c_2 \\ c_5 & c_4 & c_3 \\ c_6 & c_5 & c_4 \end{vmatrix}; \qquad D_1 = \begin{vmatrix} -c_5 & c_3 & c_2 \\ -c_6 & c_4 & c_3 \\ -c_7 & c_5 & c_4 \end{vmatrix};$$

$$D_2 = \begin{vmatrix} c_4 & -c_5 & c_2 \\ c_5 & -c_6 & c_3 \\ c_6 & -c_7 & c_4 \end{vmatrix}; \qquad D_3 = \begin{vmatrix} c_4 & c_3 & -c_5 \\ c_5 & c_4 & -c_6 \\ c_6 & c_5 & -c_7 \end{vmatrix}.$$

In this work we obtained the function $t_l(p, p', k^2; g)$ for the following specific shapes of interaction potential:

1) a Woods—Saxon potential

$$g \cdot V(r) = -V_0 \cdot [1 + \exp((r - r_0)/a)]^{-1} \text{ for } 0 < r < \infty,\ g = 1;$$

2) a Gauss potential

$$g \cdot V(r) = -V_0 \cdot \exp(-r^2/r_0^2) \text{ for } 0 < r < \infty,\ g = 1.$$

For these potentials Fig. 1 shows the results of calculations for various values of $t_l(p, p', k^2; g)$, using the Pade method and Eq. (7). The variable p' in these computations was varied in the range from 0 to 4.6 m^{-1} and $p = k\ m^{-1}$. It follows from the calculations that for $p < 4\ m^{-1}$ the cubic approximation in the Pade method allows us to calculate to an accuracy of 10^{-4}. For $p > 4\ m^{-1}$ the linear approximation gives an accuracy of 10^{-4}. The results of calculations of $t_l(p, p', k^2; g)$ for all values of p, p', k^2 and the chosen potentials did not give an accuracy of 10^{-4} up to the fourth approximation, using the method of successive approximations.

Therefore, by calculating the series (7) using the Pade method, we can obtain a solution of the equation for the probability of scattering of a particle at the above potentials in the form of a rapidly convergent series. We note that terms of a series representing the solution of Eq. (4) in the Pade method can be given a physical interpretation, since they are made up of terms of the series (7) or amplitudes of the n-fold scattering.

NOTATION

p, p', wave vectors; k^2, system energy; ε, a small parameter; $i = \sqrt{-1}$; $\mathbf{r}$, radius vector; Ω_1, wave vector space; Ω_2, radius vector space; V_0, depth of potential; a, smearing parameter; r_0, radius of the potential well.

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EFFECTIVE THERMAL AND ELECTRICAL CONDUCTIVITIES OF ANISOTROPIC DISPERSED MEDIA

R. Z. Grinberg, A. D. Terekhov, and É. M. Sher

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We obtain formulas for determining the principal values of the thermal-conductivity and electrical-conductivity tensors of materials obtained by the pressing of a powder consisting of anisotropic grains.

Present-day industry makes extensive use of a number of materials obtained by pressing of a powder consisting of anisotropic particles. Thus, for example, the branches of thermoelements used in refrigerators and generators are obtained by pressing pulverized ternary alloys with a Bi_2Te_3 base [1] which have strong anisotropy in the original (single-crystal) state.

Even though the powder is isotropic before pressing, after the pressing it displays anisotropic properties, although to a lesser degree than in a single crystal. These phenomena were mentioned in [2-4]. The authors of those studies attributed the phenomenon to the presence of microcracks.

However, an explanation of the anisotropy phenomenon on the basis of microcracks alone is unjustified. In [5] it was shown that the anisotropy in thermal conductivity and electrical conductivity that may arise as a result of porosity in the pressing process is much lower than the observed value, and, consequently, cracks alone cannot explain the anisotropy. It should also be noted that in [2], although the anisotropy was attributed to the presence of microcracks, it was stated outright that no microcracks were observed. In [4] it is noted that specimens made of pressed material have a "visible texture," indicating the presence of a certain degree of disorder in the dispersed particles which results from pressing.

We shall show below that the anisotropy of pressed specimens can be completely explained by the appearance of a degree of disorder in the orientation of the dispersed particles with respect to the direction of pressing.

For this purpose, we shall derive relations for the effective thermal conductivity $\varkappa_{eff}$ and the effective electrical conductivity σ_{eff} of a dispersed material consisting of anisotropic particles.

We shall solve the problem for the following assumptions.

1. In deriving the relation, we shall start from the fundamental assumption that a dispersed medium is a system of chaotically arranged anisotropic particles whose orientation is characterized by a differential distribution function with respect to some direction.

2. At distances much greater than the dimensions of the individual grains the dispersed medium is spatially homogeneous.

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