A SOLUTION OF THE KINETIC EQUATION FOR THE PROPAGATION OF RADIATION IN NANODISPERSED ABSORBING MEDIUM IN THE APPROXIMATION OF SMALL SCATTERING ANGLES

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Abstract: An analytic solution of the kinetic equation for the propagation of radiation (photons, neutrons) in nanodispersed absorbing medium is derived in the approximation of small scattering angles.

The main feature of the propagation of radiation (photons, neutrons) with a wavelength $\lambda \sim$ 0,1-1 nm in nanodispersed media with a typical size of dispersed particles $a \sim$ 1-10 nm in comparison with the conventional (solid) substance is that the radiation undergoes additional intense coherent elastic scattering on dispersed particles. Coherent scattering is substantially the diffraction of radiation on the dispersed nanoparticle. A single-scattering angle ϑ_1 is limited to a certain maximum angle: $\vartheta_1 \le \vartheta_{\max} \sim \lambda\!\!\!^{-} / a$, where $\lambda\!\!\!^{-} = \lambda/(2\pi)$. In some cases of practical importance the basic processes of the interaction of radiation with nanodispersed media are radiation absorption by matter and coherent elastic scattering on dispersed nanoparticles.

We assume for medium a simple structural model: equivalent round nanoparticles with a radius a; the particle density in the medium is N_0 (fig. 1). A sample of the nanodispersed material is shaped in the form of a plate of a thickness L.

We consider the following geometry. A broad homogeneous beam of radiation with a wavelength λ falls along the normal to the surface (along the axis z) of a plane nanodispersed layer with a thickness L. Using the condition of smallness of the angle of single scattering of radiation on a single nanoparticle $\vartheta_1 \sim \lambda\!\!\!^{-} / a << 1$, we write the equation of radiation propagation in nanodispersed medium in the differential form (flat geometry, fig. 1) [1–3]:

$$\mu \frac{\partial I(z,\mu)}{\partial z} = -\Sigma_a I(z,\mu) + \frac{\langle \theta_s^2 \rangle}{4} \left[\frac{\partial}{\partial \mu} \left(1-\mu^2\right) \frac{\partial I(z,\mu)}{\partial \mu} \right]. \tag{1}$$

Here $I(z,\mu) = v_0 f(z,\mu)$ is the flux density of radiation (photons, neutrons) with a wavelength λ and the propagation direction $\mathbf{\Omega}$ at the depth z in the nanodispersed medium; $f(z,\mu)$, v_0 are the distribution function and the speed of radiation particles (photons, neutrons) respectively; $\mu = \mathbf{\Omega\Omega_0} = \cos\theta$; $\mathbf{\Omega}'$, $\mathbf{\Omega}$ are unit vectors of the radiation particles before and after scattering, $\mathbf{\Omega_0}$ is unit vector of the particle velocity in the incoming radiation beam; Σ_a is the coefficient of radiation attenuation due to absorption in the medium; $\langle\theta_s^2\rangle = 2\pi\int_0^\pi \vartheta^3 w(\vartheta)\,d\vartheta$ is the mean square of the angle of scattering of radiation with a wavelength λ per unit length; $w(\vartheta)\,d\vartheta = N_0 d\sigma(\vartheta)$ is the probability of scattering of radiation with a wavelength λ to an angle $\vartheta = \arccos(\mathbf{\Omega}'\mathbf{\Omega})$ per unit length; ϑ is the angle between the unit vectors of the velocity of radiation particles $\mathbf{\Omega}'$ and $\mathbf{\Omega}$ before and after the scattering of radiation on a nanoparticle; $d\sigma(\vartheta)$ is the differential cross section of elastic coherent scattering of radiation with a wavelength λ on a dispersed nanoparticle.

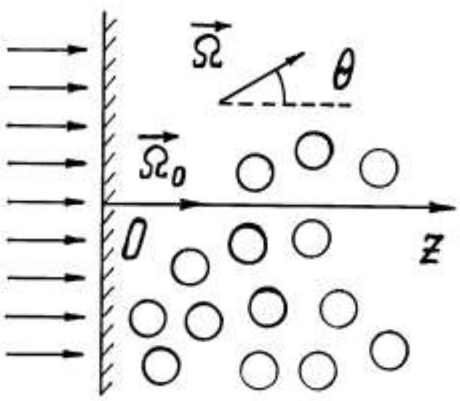

Fig. 1. A model of nanodispersed medium.

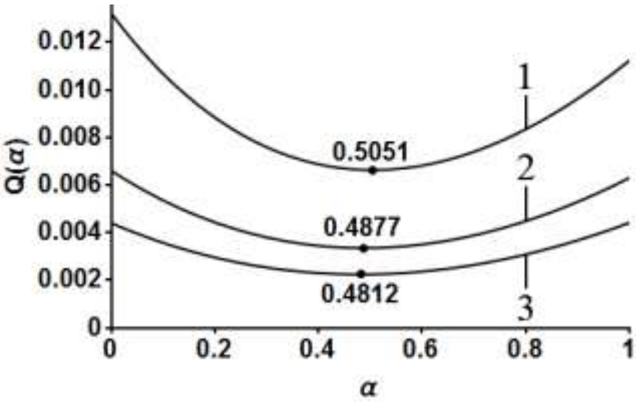

Fig. 2. Calculated values Q as a function of α parameter. 1, 2, 3 – values $\Sigma_a/\langle\theta_s^2\rangle$=10, 20, 30 respectively. Points - values α_{min}. $\rho(\xi) = \sqrt{\xi}$.

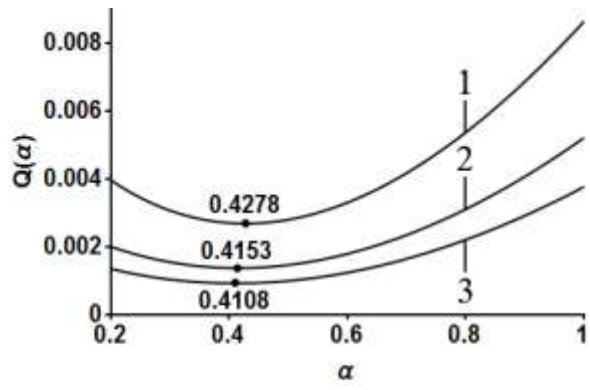

Fig. 3. Calculated values Q as a function of α parameter. 1, 2, 3 – values $\Sigma_a/\langle\theta_s^2\rangle$=10, 20, 30 respectively. Points - values α_{min}. $\rho(\xi) = \sqrt{\xi}$.

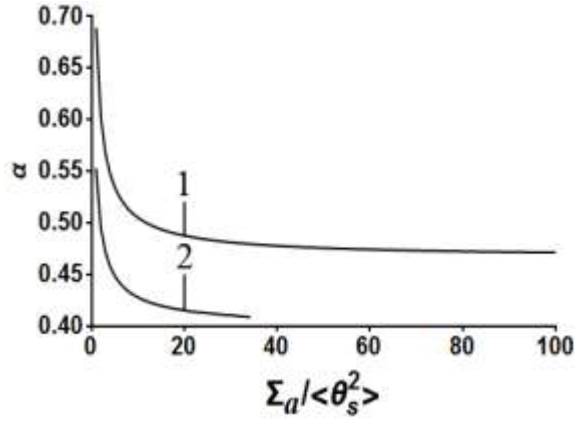

Fig. 4. Calculated values α_{min} as a function of parameter $\Sigma_a/\langle\theta_s^2\rangle$. 1 – $\rho(\xi) = \sqrt{\xi}$; 2 – $\rho(\xi) = \xi$

Because of the symmetry of the problem, the distribution function $f(z,\mu)$ of the radiation particles does not depend on *x* and *y* coordinates and the azimuth angle φ (flat geometry), and is determined only by the depth *z* and the angle θ of deviation from the initial direction $\mathbf{\Omega_0}$ of the radiation beam. Considering the ratio $\frac{\partial}{\partial\mu}\left(1-\mu^2\right)\frac{\partial I(z,\mu)}{\partial\mu} = \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial I(z,\theta)}{\partial\theta} = \Delta_\theta I(z,\theta)$, where $\mu=\cos\theta$; Δ_θ is the Laplace operator in spherical coordinates, the transport equation (1) can be written in the diffusion approximation:

$$\mu\frac{\partial I(z,\theta)}{\partial z} = -\Sigma_a I(z,\theta) + \frac{\langle\theta_s^2\rangle}{4}\Delta_\theta I(z,\theta). \qquad (2)$$

The diffusion equation (2) describes the change in the radiation distribution function through the process of diffusion of directions of radiation propagation in the space of scattering angles θ. The boundary conditions on the surfaces of the plate of the nanodispersed medium with a thickness *L* have the form:

$$I(z=0,\mu) = \{\ (I_0/2\pi)\cdot\delta(1-\mu),\ \text{for}\ 0<\mu<1\ \big|\ I_1(\mu),\ \text{for}\ -1<\mu<0\ \}, \qquad (3)$$

$$I(z=L,\mu) = \{\ I_2(\mu),\ \text{for}\ 0<\mu<1\ \big|\ 0,\ \text{for}\ -1<\mu<0\ \}, \qquad (4)$$

where I_0 is the flux density of the incident radiation. The function $I_1(\mu)$ determines the angular spectrum of the reflected radiation, the function $I_2(\mu)$ determines the angular spectrum of radiation passing through the plate.

For a small plate thickness *L*, the probability of deviation of radiation to large angles is negligible, and the mean square radiation scattering angle is small: $\langle\theta^2\rangle_L << 1$. For thick plates of absorbing medium, with increasing *z* coordinate the distribution function $f(z,\theta)$ for large values of angle θ decreases exponentially as a result of additional attenuation. The additional exponential weakening is due to the increase in the optical path length of radiation propagation in the material at high scattering angles θ. This means that the distribution $I(z,\theta)$ is significantly different from zero only for small angles ($\theta << 1$). The smallness of the angle of multiple radiation scattering can simplify the problem (2)-(4).

The diffusion approximation involves consistent inclusion of small terms, up to $\sim\theta^2$, into the equations. Therefore one assumes $\mu = \cos\theta \cong 1 - \theta^2/2 \cong (1 + \theta^2/2)^{-1}$ in the equation (2). $\sin\theta \cong \theta$ is replaced in the Laplace operator.

Since the solution $I(z,\theta)$ should decrease rapidly with the increase of θ, we can formally define the range of variation $0 \le \theta < \infty$ and require $I(z,\theta)\longrightarrow 0$ at $\theta\longrightarrow\infty$. At normal incidence of radiation the diffusively reflected flux is absent, that is $I_1(\theta) = 0$ in (3).

As a result of transformations we find that for small-angle scattering, the radiative propagation equation in the diffusion approximation with the boundary conditions (2)-(4) takes the form:

$$\frac{\partial I(z,\theta)}{\partial z} = -\left(1+\frac{\theta^2}{2}\right)\Sigma_a I(z,\theta) + \frac{\langle\theta_s^2\rangle}{4}\left(1+\frac{\theta^2}{2}\right)\left[\frac{1}{\theta}\frac{\partial}{\partial\theta}\left(\theta\frac{\partial I(z,\theta)}{\partial\theta}\right)\right], \qquad (5)$$

$$I(z=0,\theta) = \frac{I_0}{2\pi}\frac{\delta(\theta)}{\theta}, \qquad I(z,\theta)=0 \quad \text{for } \theta \longrightarrow \infty. \qquad (6)$$

Let us analyze the problem (5)-(6). In the initial statement of the problem (2)-(4) there were three characteristic length parameters: L – thickness of the plate material; $l_a = 1/\Sigma_a$ – mean free path of the radiation particles till their absorption in the medium; $l_{tr} \cong 2\left(\langle\theta_s^2\rangle\right)^{-1}$ – transport length of the coherent elastic scattering of radiation by nanoparticles. The parameter L was used in the condition $\langle\theta^2\rangle_L << 1$; it is not explicitly included in the obtained equations (5)-(6).

For the material with low absorption of radiation, the relation $l_a >> l_{tr}$ is valid, and terms containing the factor Σ_a can be neglected in the equation (5). For values $z > l_{tr}$, the equation (5) cannot be used, and the diffusion equation in coordinate space should be solved for describing the propagation of radiation in nanodispersed materials. For values $z << l_{tr}$, the equation (5) reduces to the well-known equation of propagation of radiation in matter without being absorbed [1]: $\partial I(z,\theta)/\partial z = \frac{\langle\theta_s^2\rangle}{4}\left[\frac{1}{\theta}\frac{\partial}{\partial\theta}\left(\theta\frac{\partial I(z,\theta)}{\partial\theta}\right)\right]$. For the boundary conditions (6), we obtain its solution for $z << l_{tr}$: $I(z,\theta) = I_0\left(\pi z\langle\theta_s^2\rangle\right)^{-1}\exp\left[-\theta^2/\left(z\langle\theta_s^2\rangle\right)\right]$. The condition of applicability of this solution at small depths will be $z >> l_s$, where $l_s = (N_0\sigma)^{-1}$ is the mean free path of the radiation in the material before scattering; σ is the total cross section of elastic coherent scattering of radiation with a wavelength λ on a dispersed nanoparticle.

Otherwise, for a material with strong absorption of radiation the following relation is valid:

$$l_a << l_{tr}, \quad \text{or} \quad l_a\langle\theta_s^2\rangle/2 << 1. \qquad (7)$$

In this case, the equation (5) reduces to the equation $\partial I(z,\theta)/\partial z = -\Sigma_a I(z,\theta)$, with the solution $I(z) = I_0\exp(-\Sigma_a z)$ for $z \geq 0$. The condition (7) points to the applicability, for absorbing materials, of the approximation of small-angle scattering of radiation for all values $z < \infty$. Therefore, it is natural to use below the following dimensionless length variable $\xi = z\Sigma_a$ for solving the problem (5)-(6).

The problem (5)-(6) will be solved using the variation method analogous to that of Ritz. We introduce the operator $\hat{T}$, which acts on some function $P(z,\theta)$ as follows:

$$\hat{T}[P(z,\theta)] = -\frac{\partial P(z,\theta)}{\partial z} - \left(1+\frac{\theta^2}{2}\right)\Sigma_a P(z,\theta) + \frac{\langle\theta_s^2\rangle}{4}\left(1+\frac{\theta^2}{2}\right)\left[\frac{1}{\theta}\frac{\partial}{\partial\theta}\left(\theta\frac{\partial P(z,\theta)}{\partial\theta}\right)\right]. \quad (8)$$

Consider the integral

$$S = \int_0^L \rho(z)dz\int_0^\infty \theta\left\{\hat{T}\left[P(z,\theta)\right]\right\}^2 d\theta. \quad (9)$$

For absorbing materials, it is possible to assume in many cases $L\longrightarrow\infty$, and consider the problem for the half-space $z\geq 0$. Integral S in the weight function $\rho(z)\geq 0$ is non-negative and vanishes only if the function $P(z,\theta)$ meets the transport equation (5). Thus, solving the transport equation (5) is equivalent to the requirement that the value of S have to has the minimum possible value. If the function $P_0(z,\theta)$ is an exact solution of the equation (5), then $\hat{T}[P_0(z,\theta)]\equiv 0$ and $\hat{T}\left[F(z,\theta)-P_0(z,\theta)\right]\equiv\hat{T}\left[F(z,\theta)\right]$ for any function $F(z,\theta)$. By approximating the function $P_0(z,\theta)$ with any suitable function $F(z,\theta)$, in which there are parameters with undetermined values, and substituting the function $F(z,\theta)$ in the expression (9), we obtain an approximate solution of the transport equation meeting the requirement $\delta S = 0$. Equations (8)-(9) provide the smallest squared deviation, with a weight $\rho(z)$, of the approximate function $F(z,\theta)$ from the exact solution $P_0(z,\theta)$ of the transport equation.

Taking into account the results of [2, 3], we choose an approximating function to solve the equation (5) with one dimensionless variable α as follows:

$$F(z,\theta,\alpha) = \frac{\exp(-\Sigma_a z)}{z\langle\theta_s^2\rangle}\exp\left(-\Sigma_a z\theta^2\alpha\right)\exp\left[-\frac{\theta^2}{z\langle\theta_s^2\rangle}\right]. \quad (10)$$

Function

$$I(z,\theta,\alpha) = I_0 F(z,\theta,\alpha)/\pi \quad (11)$$

meets the boundary conditions (6) for $\alpha\geq 0$. By finding the numerical value of the parameter α_{min}, at which the minimum of the integral S (9) is achieved, we obtain an approximate solution of the transport equation (5) in the form $I(z,\theta,\alpha_{min})$ (10)-(11), meeting the requirement $\delta S = 0$.

Let us compute $\hat{T}[F(z,\theta,\alpha)]$. For further references, we write down the explicit calculation result up to the small terms of the order of $\sim \theta^2$ inclusive. Designating the calculation result through function $T(z,\theta,\alpha)$, taking into account (8), (10), we get:

$$T(z,\theta,\alpha) = \hat{T}\left[F(z,\theta,\alpha)\right] \cong \exp\left(-\Sigma_a z\right) \exp\left(-\Sigma_a z \theta^2 \alpha\right) \exp\left[-\frac{\theta^2}{z\langle\theta_s^2\rangle}\right] t(z,\theta,\alpha), \quad (12)$$

where

$$t(z,\theta,\alpha) = -\alpha\Sigma_a - \frac{\theta^2\Sigma_a}{2z\langle\theta_s^2\rangle} + \frac{3\theta^2\Sigma_a\alpha}{z\langle\theta_s^2\rangle} - \frac{\theta^2}{2z^2\langle\theta_s^2\rangle} - \frac{\theta^2}{2}\alpha\Sigma_a + \theta^2\alpha^2(\Sigma_a)^2 z. \quad (13)$$

For the approximate solution $I(z,\theta,\alpha_{\min})$ of the transport equation (5), we will start to finding the minimum of the integral $S(\alpha)$ with the weight $\rho(z)\geq 0$ for the parameter values $\alpha > 0$. For $L \longrightarrow \infty$ we get $S(\alpha) = \int_0^\infty \rho(z)dz \int_0^\infty \theta\left[T(z,\theta,\alpha)\right]^2 d\theta$.

It is convenient to carry out the calculation $S(\alpha)$ in two steps. We introduce notations: $y = \theta^2$, $Z(z,\alpha) = \int_0^\infty \theta\left[T(z,\theta,\alpha)\right]^2 d\theta = \frac{1}{2}\int_0^\infty \left[T(z,y,\alpha)\right]^2 dy$, and $S(\alpha) = \int_0^\infty \rho(z) Z(z,\alpha) dz$.

From (12)-(13) we get:

$$\left[T(z,y,\alpha)\right]^2 = \exp\left(-2\Sigma_a z\right) \exp\left[-2\left(\Sigma_a z\alpha + \frac{1}{z\langle\theta_s^2\rangle}\right)y\right] t_2(z,y,\alpha); \quad (14)$$

$$t_2(z,y,\alpha) = \alpha^2\Sigma_a{}^2 + \alpha^2\Sigma_a{}^2 y + \frac{\alpha^2\Sigma_a{}^2}{4}y^2 + \frac{y^2}{4\left(\langle\theta_s^2\rangle\right)^2 z^4} - \alpha^3\Sigma_a{}^3 z y^2 + \frac{\Sigma_a}{2\left(\langle\theta_s^2\rangle\right)^2 z^3}y^2 - \frac{\alpha^2\Sigma_a{}^3}{\langle\theta_s^2\rangle}y^2 +$$

$$+\frac{6\alpha^3\Sigma_a{}^3}{\langle\theta_s^2\rangle}y^2 + \alpha^4\Sigma_a{}^4 z^2 y^2 - 2\alpha^3\Sigma_a{}^3 z y + \frac{\Sigma_a{}^2}{4\left(\langle\theta_s^2\rangle\right)^2 z^2}y^2 + \frac{\alpha\Sigma_a{}^2}{2\langle\theta_s^2\rangle z}y^2 - \frac{6\alpha^2\Sigma_a{}^2}{\langle\theta_s^2\rangle z}y - \frac{3\alpha\Sigma_a{}^2}{\left(\langle\theta_s^2\rangle\right)^2 z^2}y^2 +$$

$$+\frac{\alpha\Sigma_a}{\langle\theta_s^2\rangle z^2}y - \frac{4\alpha^2\Sigma_a{}^2}{\langle\theta_s^2\rangle z}y^2 + \frac{9\alpha^2\Sigma_a{}^2}{\left(\langle\theta_s^2\rangle\right)^2 z^2}y^2 + \frac{\alpha\Sigma_a{}^2}{\langle\theta_s^2\rangle z}y + \frac{\alpha\Sigma_a}{2\langle\theta_s^2\rangle z^2}y^2 - \frac{3\alpha\Sigma_a}{\left(\langle\theta_s^2\rangle\right)^2 z^3}y^2. \quad (15)$$

Considering expressions (14)-(15), the function $Z(z,\alpha)$ is calculated analytically using the known relation $\int_0^\infty y^n \exp(-Gy)dy = n!/G^{n+1} = \Gamma(n+1)/G^{n+1}$. General constant factors in the formula $S(\alpha)$ do not affect the value of the dimensionless parameter $\alpha_{\min}$, at which the minimum of the integral $S(\alpha)$ is achieved.

We introduce the dimensionless function $b(\alpha)=\sqrt{\Sigma_a/\left(\langle\theta_s^2\rangle\alpha\right)}$, use the dimensionless variable $\xi=z\Sigma_a$ and group terms in the derived expression for $Z(z,\alpha)$. We omit common constant terms in the expression $S(\alpha)$, and get dimensionless function $Q(\alpha)$: $S(\alpha)\sim Q(\alpha)$, for which we find the minimum and evaluate α_{min}. As a result of transformations we obtain:

$$Q(\alpha) = (\alpha/2)\,K_1(\alpha)+K_2(\alpha)/4+\left\{(16\alpha)^{-1}-[b(\alpha)]^2/4+(3\alpha/2)[b(\alpha)]^2\right\}K_3(\alpha)+$$

$$+[b(\alpha)]^4(16\alpha)^{-1}K_4(\alpha)-K_5(\alpha)/4+\left[(8\alpha)^{-1}-3/4\right][b(\alpha)]^4K_6(\alpha)+(\alpha/4)\,K_7(\alpha)-$$

$$-(\alpha/2)\,K_8(\alpha)+\left\{[b(\alpha)]^4(16\alpha)^{-1}-(3/4)[b(\alpha)]^4+(9\alpha/4)[b(\alpha)]^4+[b(\alpha)]^2(8\alpha)^{-1}\right\}K_9(\alpha)+$$

$$+\left[(8\alpha)^{-1}-1\right][b(\alpha)]^2K_{10}(\alpha)+\left[(1/4)-(3\alpha/2)\right][b(\alpha)]^2K_{11}(\alpha)+[b(\alpha)]^2K_{12}(\alpha)/4\,.$$

Here we introduced the following notations:

$$K_1(\alpha)=\int_0^\infty d\xi\;\rho(\xi)\xi\exp(-2\xi)\left\{\xi^2+[b(\alpha)]^2\right\}^{-1};\quad K_2(\alpha)=$$

$$\int_0^\infty d\xi\;\rho(\xi)\xi^2\exp(-2\xi)\left\{\xi^2+[b(\alpha)]^2\right\}^{-2};\quad K_3(\alpha)=\int_0^\infty d\xi\;\rho(\xi)\xi^3\exp(-2\xi)\left\{\xi^2+[b(\alpha)]^2\right\}^{-3};$$

$$K_4(\alpha)=\int_0^\infty d\xi\;\rho(\xi)\xi^{-1}\exp(-2\xi)\left\{\xi^2+[b(\alpha)]^2\right\}^{-3};\quad K_5(\alpha)=$$

$$\int_0^\infty d\xi\;\rho(\xi)\xi^4\exp(-2\xi)\left\{\xi^2+[b(\alpha)]^2\right\}^{-3};\quad K_6(\alpha)=\int_0^\infty d\xi\;\rho(\xi)\exp(-2\xi)\left\{\xi^2+[b(\alpha)]^2\right\}^{-3};$$

$$K_7(\alpha)=\int_0^\infty d\xi\;\rho(\xi)\xi^5\exp(-2\xi)\left\{\xi^2+[b(\alpha)]^2\right\}^{-3};\quad K_8(\alpha)=$$

$$\int_0^\infty d\xi\;\rho(\xi)\xi^3\exp(-2\xi)\left\{\xi^2+[b(\alpha)]^2\right\}^{-2};\quad K_9(\alpha)=\int_0^\infty d\xi\;\rho(\xi)\xi\exp(-2\xi)\left\{\xi^2+[b(\alpha)]^2\right\}^{-3};$$

$$K_{10}(\alpha)=\int_0^\infty d\xi\;\rho(\xi)\xi^2\exp(-2\xi)\left\{\xi^2+[b(\alpha)]^2\right\}^{-3};\quad K_{11}(\alpha)=$$

$$\int_0^\infty d\xi\;\rho(\xi)\xi\exp(-2\xi)\left\{\xi^2+[b(\alpha)]^2\right\}^{-2};\; K_{12}(\alpha)=\int_0^\infty d\xi\;\rho(\xi)\exp(-2\xi)\left\{\xi^2+[b(\alpha)]^2\right\}^{-2}.$$

For the weighting function of a type $\rho(\xi)=\xi^\gamma$ for $\gamma>0$, integrals $K_1(\alpha)$, ... , $K_{12}(\alpha)$ can be calculated analytically. The minimum $Q(\alpha)$ is defined for the following weight functions: $\rho_1(\xi)=\xi$ and $\rho_2(\xi)=\sqrt{\xi}$, for $\xi\geq 0$.

With the weight functions $\rho_1(\xi)$, $\rho_2(\xi)$, integrals $K_1(\alpha), \dots, K_{12}(\alpha)$ and $Q(\alpha)$ in this paper have been calculated in an explicit analytic form.

For values of the dimensionless parameter $\Sigma_a / \langle \theta_s^2 \rangle$ in the range from 1 to 100, local minima of the function $Q(\alpha)$ were found and values of the parameter α_{min} were directly numerically calculated. Figs. 2, 3 illustrate calculated values of Q as a function of parameter α. As clear from the Figs., values of Q change only slightly in the vicinity of the minimum of α_{min}. Therefore, in most cases, the value $\alpha_{min}=1/2$ can be used for approximate estimations. The value of α_{min}, calculated here precisely, confirms validity of estimations and conclusions in [2, 3].

The values of Σ_a and $\langle \theta_s^2 \rangle$ contain information about properties of concrete materials and peculiarities of the interaction of radiation with nanoparticles. Fig. 4 presents calculated values α_{min} as a function of parameter $\Sigma_a / \langle \theta_s^2 \rangle$ for weight functions $\rho_1(\xi)$ and $\rho_2(\xi)$.

Conclusion. An analytical solution of the kinetic equation for the propagation of radiation (photons, neutrons) in nanodispersed absorbing medium is derived using variation method in the approximation of small scattering angles. An approximate solution of the equation (1) for the radiation propagation has the form:

$$I(z,\theta,\alpha_{min}) = I_0 \frac{\exp(-\Sigma_a z)}{\pi z \langle \theta_s^2 \rangle} \exp\left(-\Sigma_a z \theta^2 \alpha_{min}\right) \exp\left[-\frac{\theta^2}{z \langle \theta_s^2 \rangle}\right].$$

This expression can be applied for depths $l_s << z << 2\left(\langle \theta_s^2 \rangle\right)^{-1}$ of penetration of radiation into material. For approximate calculations, the value $\alpha_{min} = \frac{1}{2}$ can be used.

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