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D. R. YAFAEV

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ECOLE POLYTECHNIQUE

F-91128 PALAISEAU Cedex (France)

Tél. (1) 69.41.82.00

Télex ECOLEX 691.596 F

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ÉQUATIONS AUX DÉRIVÉES PARTIELLES

ON THE QUASI-CLASSICAL ASYMPTOTICS
OF THE FORWARD SCATTERING AMPLITUDE
AND OF THE TOTAL SCATTERING CROSS-SECTION

D.R. YAFAEV

One considers the Schrödinger equation with a potential vanishing asymptotically as a homogeneous function of a negative degree at infinity. The asymptotic formulas for the forward scattering amplitude and for the total scattering cross-section are derived. These formulas are valid for high energies K^2 and large coupling constants g if, moreover, $gK^{-1} \rightarrow \infty$.

1. We start by an operator definition of the amplitude of scattering by a potential $q(x)$. Let $H_0 = -\Delta$, $H = -\Delta + q(x)$, $q = \bar{q}$, be self-adjoint operators in the space $\mathcal{H} = L^2(\mathbf{R}^d)$, $d \geq 2$, and $q(x) = O(|x|^{-\alpha})$, $\alpha > 1$, as $|x| \rightarrow \infty$. Then the strong limits

$$W_{\pm} = W_{\pm}(H, H_0) = s - \lim_{t \rightarrow \pm\infty} \exp(iHt) \exp(-iH_0t)$$

exist and are called wave operators. Since $HW_{\pm} = W_{\pm}H_0$, the scattering operator $\mathcal{S} = W_{+}^{*}W_{-}$ commutes with H_0 . Consider now the representation

$$L^2(\mathbf{R}^d) \leftrightarrow L^2(\mathbf{R}_{+}; L^2(\mathbf{S}^{d-1}))$$

which is defined by the relation

$$f(x) \leftrightarrow \tilde{f}(\lambda; \omega) = 2^{-1/2} \lambda^{\frac{d-2}{4}} \hat{f}(\sqrt{\lambda}\omega)$$

with \hat{f} being the Fourier transform of f . This representation diagonalizes H_0 so that \mathcal{S} acts there as a multiplication by an operator-function $S(\lambda) = S(H, H_0; \lambda) : L_2(\mathbf{S}^{d-1}) \rightarrow L_2(\mathbf{S}^{d-1})$ which is called the scattering matrix. If $2\alpha > d + 1$ the operator $S(\lambda) - I$ is an integral operator with a kernel denoted by

$$i(K/2\pi)^{d-1} f(\varphi, \omega; K),$$

where $K = \lambda^{1/2}$ is a wave number. The function $f(\varphi, \omega; K)$ is called the amplitude of scattering in the direction φ for the direction ω of the incident beam of particles of an energy K^2 .

Another definition of the scattering amplitude may be given in terms of the Schrödinger equation

$$(1) \quad -\Delta\psi + q(x)\psi = K^2\psi.$$

If

$$(2) \quad |q(x)| \leq C(1 + |x|)^{-\alpha}$$

with $\alpha > d$, then for every $K > 0$ and every $\omega \in \mathbf{S}^{d-1}$ there exists unique solution of (1) such that

$$(3) \quad \psi(x, \omega, K) = \exp(iK\langle \omega, x \rangle) + F(\hat{x}, \omega, K)|x|^{-\frac{d-1}{2}} \exp(iK|x|)$$

$$+0(|x|^{-\frac{d-1}{2}}), \hat{x} = x|x|^{-1}, |x| \rightarrow \infty.$$

Function F and f are related by

$$F(\varphi, \omega; K) = (K/2\pi)^{\frac{d-1}{2}} \exp(-\pi i(d-3)/4) f(\varphi, \omega; K),$$

and F is also called the scattering amplitude.

In terms of F the total scattering cross-section is defined by

$$\sigma(\omega; K) = \int_{\mathbf{S}^{d-1}} |F(\varphi, \omega; K)|^2 d\varphi.$$

Under the assumption (2) with $\alpha > d$ the scattering amplitude is a continuous function of φ, ω and K so that the forward amplitude $f(\omega, \omega; K)$ is correctly defined. It is connected with $\sigma(\omega; K)$ by the so-called optical theorem

$$(4) \quad \sigma(\omega; K) = 2 \operatorname{Im} f(\omega, \omega; K),$$

which is a consequence of unitarity of $S(\lambda)$. The total scattering cross-section $\sigma(\omega; K)$ is finite if $2\alpha > d + 1$. We emphasize that

$$\int_{\mathbf{S}^{d-1}} \sigma(\omega; K) d\omega = (K/2\pi)^{-d+1} \|S(\lambda) - I\|_{HS}^2, \quad \lambda = K^2,$$

with $\|\cdot\|_{HS}$ being the Hilbert-Schmidt norm. Thus the integral of $\sigma(\omega; K)$ over ω has an invariant meaning though definitions of $f(\omega, \omega; K)$ and $\sigma(\omega; K)$ depend on the representation of \mathcal{H} .

2. Replacing $q(x)$ by $gq(x)$ we introduce a coupling constant g into notation. We shall keep track of the dependence of various objects on g , e.g. we denote $f(\varphi, \omega; K, g)$. The aim of the present talk is to describe asymptotics of $f(\omega, \omega; K, g)$ and $\sigma(\omega; K, g)$ as $K \rightarrow \infty$ and $g \rightarrow \infty$. Note that according to (4) results on the forward scattering amplitude $f(\omega, \omega; k, g)$ are more general than those on $\sigma(\omega; k, g)$. Moreover, if $\alpha \in]\frac{d+1}{2}, d]$ the total scattering cross-section is finite though $f(\omega, \omega; K, g)$ does not have sense.

Now we describe briefly some well known results. We begin with a case $K \rightarrow \infty$, $g \rightarrow \infty$, $N := g(2K)^{-1} \rightarrow 0$ when the perturbation theory (or the Born approximation in physics terms [La-Li]) can be applied. Denote by Λ_ω a plane which is orthogonal to ω , decompose each $x \in \mathbf{R}^d$ into a sum $x = z\omega + b$ with $z = \langle \omega, x \rangle$, $b \in \Lambda_\omega$ and set

$$(5) \quad V_\omega(b; q) = \int_{-\infty}^{\infty} q(z\omega + b) dz,$$

Then as shown in [Hu], [Bu], [Je] under the assumption (2)

$$(6) \quad \begin{cases} f(\omega, \omega; K, g) \sim -N \int_{\Lambda_\omega} V_\omega(b; q) db, & \alpha > d, \\ \sigma(\omega; K, g) \sim N^2 \int_{\Lambda_\omega} V_\omega^2(b; q) db, & 2\alpha > d + 1. \end{cases}$$

as $K \rightarrow \infty, g \rightarrow \infty$ and $N \rightarrow 0$.

In the region $N \rightarrow \infty$ (or in the intermediary case $N = \text{const}$) the asymptotics of f and σ can not be studied by the perturbation theory. Moreover, if $N \rightarrow \infty$ these asymptotics are expected to be very sensitive to the behavior of $q(x)$ at infinity. For a potential $q(x)$ with a compact support it was conjectured (see e.g. [En-Si]) that

$$\sigma(\omega; K, g) \rightarrow 2\sigma_{cl}(\omega)$$

as $g = cK^2 \rightarrow \infty, c = \text{const}$ this is, clearly, equivalent to the quasi-classical limit when the Planck constant $h \rightarrow 0$ and other parameters are fixed. Here a classical scattering cross-section $\sigma_{cl}(\omega)$ is by definition a \mathbf{R}^{d-1} -measure of the orthogonal projection of $\text{supp } q$ onto Λ_ω . This conjecture was proved in an averaged (over K) sense in [Yaj]. The averaging was removed in [Ro-Ta,2] where, however, the so-called non-trapping condition on the corresponding classical system was required.

3. Let us consider now the simplest case $N = \text{const}$ when the perturbation theory can not be applied. Set

$$(7) \quad \begin{cases} A(\omega; q) = i \int_{\Lambda_\omega} [1 - \exp(-iV_\omega(b; q))] db, \\ A_0(\omega; q) = 4 \int_{\Lambda_\omega} \sin^2[2^{-1}V_\omega(b; q)] db, \end{cases}$$

with $V_\omega(b; q)$ defined by (5).

Theorem 1.— Suppose that q is continuous, twice differentiable with respect to $|x|$ and functions $|x|^K |\partial^K q / \partial |x|^K|$ for $K = 1, 2$ are bounded. Let also condition (2) be fulfilled. Then for each fixed N there exist finite limits

$$(8) \quad \begin{cases} \lim_{K \rightarrow \infty} f(\omega, \omega; K, 2NK) = A(\omega; Nq), \alpha > d, \\ \lim_{K \rightarrow \infty} \sigma(\omega; K, 2NK) = A_0(\omega; Nq), 2\alpha > d + 1, \end{cases}$$

which are uniform in $N \leq N_0 < \infty$.

The detailed proof of this theorem can be found in [Yaf,2]. It is based on the so-called eikonal approximation. Roughly speaking, this means that the function $\psi(x, \omega, K, g)$ defined by (1), (3) has the asymptotics

$$\exp[iK \langle \omega, x \rangle - iN \int_{-\infty}^z q(z'\omega + b) dz']$$

as $g = 2NK \rightarrow \infty, N = \text{const}$.

Note that taking $N \rightarrow 0$ one can deduce relations (6) from (8).

4. Our main goal is to discuss asymptotics of $f(\omega, \omega; K, g)$ and $\sigma(\omega; K, g)$ in the region $K \rightarrow \infty, g \rightarrow \infty$ and $N \rightarrow \infty$. We restrict ourselves to potentials $q(x)$ with an asymptotics

$$(9) \quad q(x) = |x|^{-\alpha} \varphi(\hat{x}) + o(|x|^{-\alpha}), \varphi \in C(\mathbf{S}^{d-1}),$$

at infinity. Set $\nu = (\alpha - 1)^{-1}, \rho = (d - 1)\nu, q_{as}(x) = |x|^{-\alpha} \varphi(\hat{x})$. In the paper [Bi-Yaf] it was conjectured that as $N \rightarrow \infty$ the following relations should be true

$$(10) \quad f(\omega, \omega; K, g) \sim A(\omega; q_{as}) N^\rho, \quad \alpha > d,$$

$$(11) \quad \sigma(\omega; K, g) \sim A_0(\omega; q_{as}) N^\rho, \quad 2\alpha > d + 1.$$

We shall see that these asymptotics are correct if only understood in an averaged sense. Namely, for arbitrary $\xi \in C_0^\infty(\mathbf{R})$ such that $\text{supp} \xi \subset [-1, 1]$ and $\int \xi^2(\rho) d\rho = 1$ define

$$f_\ell^{(av)}(K) = \ell^{-1} \int f(p) \xi^2(\ell^{-1}(\rho - K)) d\rho, \quad 0 < \ell < K.$$

Now we can state

Theorem 2.— *Let the condition (9) be fulfilled. Then*

$$(12) \quad f_\ell^{(av)}(\omega, \omega; K, g) \sim A(\omega; q_{as}) N^\rho, \quad \alpha > d,$$

$$(13) \quad \sigma_\ell^{(av)}(\omega; K, g) \sim A_0(\omega; q_{as}) N^\rho, \quad 2\alpha > d + 1,$$

as

$$(14) \quad N \rightarrow \infty, gK^{\alpha-2} \rightarrow \infty$$

and

$$\ell N^\nu \rightarrow \infty, \ell = o(K).$$

Let us make some comments on this theorem. The region (14) where (12), (13) hold true depends on α but not on d . Clearly, this region becomes larger the smaller α is. The quasi-classical ($g = cK^2, c = \text{const}$ and large coupling constant ($g \rightarrow \infty, K$ fixed) limits are always permitted. In case $\alpha \geq 2$ in the region (14) g should tend to infinity but it is permitted that $K \rightarrow 0$ if only $gK^{\alpha-2} \rightarrow \infty$. Moreover, in case $\alpha \in (3/2, 2), d = 2$ the asymptotic formula (13) is true even for $K \rightarrow 0, g$ fixed (i.e. in a low energy limit).

Assumptions on an averaging parameter ℓ are of a technical nature. Clearly, the result is stronger if ℓ is smaller. We permit that ℓ tends to zero but not too quickly.

We do not have any local assumptions on q . If q is bounded only for large $|x|$, i.e. for $x \notin B$ where B is some ball, then the Hamiltonian $H_g = -\Delta + gq(x)$ should be defined as an arbitrary self-adjoint operator for which

$$(15) \quad H_g u = -\Delta u + gq(x)u, u \in C_0^\infty(\mathbf{R}^d \setminus B).$$

Such Hamiltonians certainly exist but are not unique. In the ball B a perturbation is quite arbitrary and it is not even required that it should be an operator of multiplication. For example, in addition to q satisfying (9) we permit perturbations of H_0 by differential operators of arbitrary order if their coefficients have compact supports. In such cases wave operators $W_{\pm}(H_g, H_0)$ exist but the stationary method of their construction can not be applied and the unitarity of the scattering matrix $S(H_g, H_0, \lambda)$ may be violated. In this singular situation only the first (time-dependent) definition of $f(\varphi, \omega; K, g)$ makes sense. Relations (12), (13) hold true for f and σ defined by a scattering matrix $S(H_g, H_0; \lambda)$ for any self-adjoint H_g obeying (15).

The proof of the upper bound for $\sigma^{(av)}$ with the correct power N^ρ was obtained in [Am-Pe] and [En-Si]. To that end only the upper bound (2) for q is required. Under this assumption it is possible also to prove that

$$|f_\ell^{(av)}(\varphi, \omega', K, g)| \leq CN^\rho, \varphi, \omega \in \mathbf{S}^{d-1}.$$

In the paper [Bi-Yaf] relations (10), (11) were derived from the asymptotics for large numbers of eigenvalues of $S(H_g, H_0; \lambda)$ accumulating to a point 1. In [Bi-Yaf] such asymptotics was found for fixed $\lambda = u^2$ and g . If this asymptotics was justified uniformly in K and g , then similarly to a central case [La-Li] it would have ensured (10), (11) (or (12), (13)). Unfortunately such an approach to the proof of Theorem 2 seems to promise nothing.

The proof of Th.2 relies on the separate consideration of different regions of \mathbf{R}^d . It turns out that the asymptotics of f and σ are determined only by the region where $|x| \sim N^\nu$. There $q(x)$ can be replaced by $q_{as}(x)$ and the problem is reduced by scaling to the “critical” case $N = \text{const}$ studied in Th.1. The region where $|x|N^{-\nu} \rightarrow \infty$ is treated by perturbation theory. The main difficulty is to estimate the contribution to f and σ of the ball $|x| = 0(N^\nu)$. This is performed by time-dependent means and requires averaging over K . Note that for a potential supported in a ball of a radius R averaged f and σ are bounded by CR^{d-1} . Thus it is natural to expect that the difference of scattering amplitudes and scattering cross-sections for potentials which coincide outside of the ball of the radius $o(N^\nu)$ is bounded by $o(N^{\nu(d-1)}) = o(N^\rho)$. Our proof of this result is somewhat similar to that of [En-Si] but demands an introduction of an auxiliary “free” Hamiltonian. The detailed proof of Th.2 can be found in [Yaf,3].

Let us compare relations (6) and (12), (13). They are qualitatively different in two respects. First, by (6) as $N \rightarrow 0$ the forward scattering amplitude is vanishing as N and the total cross-section as N^2 , whereas by (12), (13) f and σ are growing as $N \rightarrow \infty$ with the speed determined by the fall-off of $q(x)$ at infinity. Second, as $N \rightarrow 0$ the asymptotics of f and σ depend on values of $q(x)$ for all $x \in \mathbf{R}^d$. On the contrary, as $N \rightarrow \infty$ the asymptotics of f and σ are determined only by the asymptotics of $q(x)$ at infinity.

According to Th.1 in the “critical” case $N = \text{const}$, the forward scattering amplitude and the total scattering cross-section converge as $K \rightarrow \infty$ to finite limits. As in the case $N \rightarrow 0$ these limits depend on values of $q(x)$ for all $x \in \mathbf{R}^d$ but are calculated in terms of integrals (7) as in the case $N \rightarrow \infty$.

5. The method used for the proof of Th.2 can be applied [Yaf,3] also to the high-energy scattering on strongly singular potentials when the Born approximation (6) fails to be true.

Theorem 3.— Let $|q(x)| \leq C|x|^{-\alpha}$ for $|x| \geq C > 0$ and

$$q(x) = |x|^{-\beta}\varphi(\hat{x}) + o(|x|^{-\beta}), |x| \rightarrow 0.$$

Set now $q_{as}(x) = |x|^{-\beta}\varphi(\hat{x})$, $\nu = (\beta - 1)^{-1}$, $\rho = (d - 1)\nu$. Then in the region $N \rightarrow 0$, $gK^{\beta-2} \rightarrow \infty$ the relations (12) for $\beta > d$ and (13) for $2\beta > d + 1$ are fulfilled if $\ell N^\nu \rightarrow \infty$, $\ell = o(K)$.

Compared to (6) in the singular case $f(\omega, \omega; K, g)$ and $\sigma(\omega; k, g)$ are vanishing slower as $N \rightarrow 0$ and their asymptotics are determined only by the singularity of $q(x)$ at $x = 0$.

If the potential is exactly of the form $q(x) = |x|^{-\alpha}\varphi(\hat{x})$, then the relations (12), (13) hold true in the whole region $gK^{\alpha-2} \rightarrow \infty$. The assumptions $N \rightarrow \infty$ (Th.2) or $N \rightarrow 0$ (Th.3) are required only to replace q by its asymptotics at $x = \infty$ or $x = 0$.

6. Let us return now to the study of the case $N \rightarrow \infty$. In what follows potentials are supposed to be bounded.

Without averaging the relations (10) and (11) are in general violated. Moreover, the usual point of view that for a potential with a compact support the total cross-section should be bounded by a constant depending only on the size of its support fails also to be true. It is a consequence of the following assertion [Yaf,1].

Theorem 4.— Let $q(x) = q(r)$, $x \in \mathbf{R}^3$, $r = |x|$, have a compact support and let $q(r) < 0$ on a set of a positive Lebesgue measure in \mathbf{R}_+ . Then for each $K > 0$ there exists a sequence $g_\ell = g_\ell(K) \rightarrow \infty$ as $\ell \rightarrow \infty$ such that the lower bound

$$(16) \quad \sigma(K, g_\ell) \geq Cg_\ell^{1/2}$$

holds.

Let us give an idea of the proof. Recall that for every $\ell = 0, 1, 2, \dots$ the solution of the equation

$$-y'' + \ell(\ell + 1)r^{-2}y + gq(r)y = K^2y$$

satisfying $\psi_\ell(r) = 0(r^{\ell+1})$ as $r \rightarrow 0$ has an asymptotics

$$\psi_\ell(r) \sim C_\ell \sin(Kr - 2^{-1}\pi\ell + \delta_\ell)$$

as $r \rightarrow \infty$. In terms of phase shifts $\delta_\ell = \delta_\ell(K, g)$ the total scattering cross-section is determined by the formula

$$(17) \quad \sigma(K, g) = 4\pi K^{-2} \sum_{\ell=0}^{\infty} (2\ell + 1) \sin^2 \delta_\ell(K, g).$$

Thus for the proof of Th.4 it suffices to establish :

Lemma 5.— Under the assumptions of Th.4 for all sufficiently large ℓ there exist coupling constants $g_\ell = g_\ell(K)$ such that $\delta_\ell(K, g_\ell) = \pi/2$ and $c_1\ell \leq g_\ell \leq c_2\ell^2$.

The “anormal” growth (16) of the total scattering cross-section has of course a resonant nature. Suppose that $q(r) \leq 0$ and $q(r) = 0$ for $r \geq r_1$. For orbital momentum $\ell, \ell(\ell + 1) \geq K^2 r_1^2$, the effective potential

$$(18) \quad q_{eff}(r) = \ell(\ell + 1)r^{-2} + gq(r)$$

does not allow a classical particle coming from infinity with an energy K^2 to penetrate into the region where $r^2 \leq \ell(\ell + 1)K^{-2}$. Thus for large ℓ a classical particle does not “feel” the potential well $gq(r)$ supported in $[0, r_1]$. In contrast to a classical, a quantum particle can penetrate through a barrier $\ell(\ell + 1)r^{-2}$ on account of tunneling. Thus the potential $gq(r)$ perturbs all phase shifts δ_ℓ but with the growth of the barrier the influence of $gq(r)$ is generically quickly vanishing so that $\delta_\ell(K, g)$ are small for large ℓ . However, lemma 5 shows that for every fixed $K_0 > 0$ the phase shift $\delta_\ell(K, g)$ jumps quickly to $\pi/2$ as $K \rightarrow K_0$ and $g \rightarrow g_\ell(K_0)$. This is naturally explained by the existence of the quasistationary state with an energy K_0^2 in the field of the potential (18) with $g = g_\ell(K_0)$ (cf. with Gamov’s theory discussed, for example, in the book [Ba-Ze-Pe]).

The assumption of Th.4 that q has a compact support is of course inessential. This theorem is true for all potentials obeying (2) with $\alpha > 2$. Relations (11) and (16) are incompatible if $\alpha > 5$ and $g \rightarrow \infty, K$ fixed.

7. Nevertheless, in many cases the asymptotics (10) and (11) are fulfilled without averaging. For example, it is sufficient [Yaf,2] to assume that $N \rightarrow \infty$ but gK^{-2} is small enough. The last condition was used in [Yaf,2] only to obtain the following bound for the resolvent. Let X_β be a multiplication by $(1 + |x|)^{-\beta}, \beta > 1/2$. Then the product

$$X_\beta(-\Delta + gq - K^2 - i\varepsilon)^{-1} X_\beta$$

has a norm-limit $T(K, g)$ as $\varepsilon \rightarrow 0$ and

$$(19) \quad \|T(K, g)\| \leq CK^{-1}$$

(In fact in [Yaf,2] a slightly more general bound was verified and used.) Once in some subregion of (14) the bound (19) is proven, the method of [Yaf,2] permits to obtain there the asymptotics (10), (11).

In the quasi-classical case $gu^{-2} = c = \text{const}$ the bound (19) was established in [Va] and [Ro-Ta,1,2]. In these papers c was not required to be small but the non-trapping condition was imposed. The bound (19) was used in [Ro-Ta,2] to obtain the asymptotics of $\sigma(\omega; K, g)$ in a more general form compared to (11). Namely, under certain assumptions it was shown in [Ro-Ta,2] that as $g = CK^2 \rightarrow \infty$

$$\sigma(\omega; K, g) = 4 \int_{\Lambda_\omega} \sin^2(2^{-1}NV_\omega(b; q))db + o(N^\rho).$$

It turns out that the bound (19) is not really necessary for the asymptotics (10), (11). Thus one can dispense with the assumptions on the corresponding classical system. The conditions of validity of (10), (11) were studied in [So-Yaf,1] for the central case. There the following assertion was established.

Theorem 6.— Let $q(x) = q(r)$, $x \in \mathbf{R}^3$, $r = |x|$, and $q(r) = q_0 r^{-\alpha} + o(r^{-\alpha})$ as $r \rightarrow \infty$. Then relations (10), (11) hold true in the region

$$(20) \quad N \rightarrow \infty, g^{3-\alpha} K^{2(\alpha-2)} \rightarrow \infty$$

If, moreover, $q(r) \geq 0$, then relations (10), (11) are fulfilled in the whole region (14).

Now $q_{as}(x) = q_0 |x|^{-\alpha}$ so that integrals $A(q_{as})$ and $A_0(q_{as})$ can be easily evaluated. Clearly, as (14), the region (20) becomes larger the smaller α is. The quasiclassical limit $g = cK^2$ is permitted in (20) for all α but the large coupling constant limit $g \rightarrow \infty$, k fixed, is allowed only for $\alpha \in (2, 3)$. Th.6 can be deduced from the asymptotics of phase shifts. The latter is given by the following.

Lemma 7.— Let q satisfy conditions of Th.6 and let c be any fixed positive number. Set

$$\tau_\alpha = 2^{-2} \pi^{1/2} \Gamma((\alpha - 1)/2) \Gamma^{-1}(\alpha/2).$$

Then

$$(21) \quad \sup_{\ell: (\ell + \frac{1}{2})^{\alpha-1} \geq cgK^{\alpha-2}} |\delta_\ell(K, g)(gK^{\alpha-2})^{-1} (\ell + \frac{1}{2})^{\alpha-1} + \tau_\alpha q_0| \rightarrow 0$$

in the region (20). If, moreover, $q(r) \geq 0$, then (21) holds true in the region (14).

Now the proof of Th.6 can be obtained by substituting (21) into the sum (17). Further details may be found in [So-Ya,2] and the complete proof - in [So-Ya,1]. Note that the condition $d = 3$ in Theorems 4 and 6 is of course inessential.

Under certain assumptions it was shown recently by A.V. Sobolev that the assertion similar to Th.6 holds true in the general (not necessarily central) case. In his approach σ is averaged over the incident direction ω but not over the energy.

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Dmitrij YAFAEV
LOMI, Fontanka 27
Leningrad, 191011 U.S.S.R.