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On the quasi-classical limit of the total scattering cross-section in nonrelativistic quantum mechanics

by

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ABSTRACT. — The total scattering cross-section for the operator $-\Delta + gV$ is studied for large coupling constants g and high energies K^2.

RÉSUMÉ. — La section efficace totale de diffusion pour l'opérateur $-\Delta + gV$ est étudiée pour les grandes constantes de couplage g et les hautes énergies K^2.

1. INTRODUCTION. A GENERAL SURVEY

The total scattering cross-section for the Schrödinger equation

$$-\Delta u + gV(x)u = K^2u \tag{1.1}$$

where $x \in \mathbb{R}^3$, $K > 0$, $g > 0$ and [1]

$$|V(x)| \leqslant C(1 + |x|)^{-\alpha}, \qquad \alpha > 2, \tag{1.2}$$

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[1] By C and c we denote different positive constants. If necessary, its dependence on some parameters is specified in the notation, i.e. $C = C(K)$.

can be defined in the following way. Denote by $S(K, g)$ the scattering matrix for the equation (1.1) (for the precise definition see below). Then $S(K, g) - I$ is an integral operator in the space $L_2(\mathbb{S}^2)$ with a kernel $(2\pi)^{-1} iK f(\varphi, \omega; K, g)$, $\omega \in \mathbb{S}^2$. The function f is called the amplitude of scattering in the direction φ for the direction ω of the incoming plane wave. In terms of f the total scattering cross-section for the incoming direction ω is defined by

$$\sigma(\omega; K, g) = \int_{\mathbb{S}^2} | f(\varphi, \omega; K, g) |^2 d\varphi . \tag{1.3}$$

When averaged over ω

$$\sigma(K, g) := (4\pi)^{-1} \int_{\mathbb{S}^2} \sigma(\omega; K, g) d\omega = \pi K^{-2} \| S(K, g) - I \|_2^2, \tag{1.4}$$

where $\| \, . \, \|_2$ is the Hilbert-Schmidt norm.

The aim of this paper is to discuss the asymptotic behavior of $\sigma(\omega; K, g)$ as the energy K^2 of the particle and the coupling constant g both tend to infinity. Note that the equation, formally more general than (1.1), $-\hbar^2 \Delta u + gV(x)u = K^2 u$ is obviously reducible to (1.1). In particular, the quasi-classical limit as $\hbar \to 0$, g and K fixed, is the same as that for (1.1) as $g = cK^2 \to \infty$, $c = \text{const}$. However, we do not restrict ourselves to this particular case and permit different relations between g and K as $g \to \infty$, $K \to \infty$. Though the total cross-section is one of the basic objects in a quantum scattering problem, there was little study of it until recently. Even at a heuristic level some quite general properties of $\sigma(\omega; K, g)$ seem not to be commonly known. We emphasize that the asymptotics of $\sigma(\omega; K, g)$ as $K \to \infty$, $g \to \infty$ depends crucially on the relation between K and g and on the rate of the fall-off of $V(x)$ at infinity.

We begin our discussion with the simple case when $g/K \to 0$. As is well-known (see e. g. [*1*]) as $K \to \infty$, g fixed, or $g \to 0$, K fixed, the asymptotics of different scattering characteristics for the equation (1.1) may be obtained by perturbation theory (Born approximation in physical terms). These formulae can be rigorously justified [*2*]-[*4*] and, moreover, if $g/K \to 0$ they are valid also in case $K \to \infty$, $g \to \infty$. In particular, for the total cross-section the Born approximation shows that under suitable assumptions on V:

$$\sigma(\omega; K, g) \sim (g/2K)^2 \int_{\mathbb{R}^2} db \left[\int_{-\infty}^{\infty} dz V(b + \omega z) \right]^2 , \tag{1.5}$$

where $b \in \mathbb{R}^2$, $\langle b, \omega \rangle = 0$, $x = b + \omega z$. Thus in case $g/K \to 0$ the asymptotics of $\sigma(\omega; K, g)$ depends on the values of $V(x)$ for all $x \in \mathbb{R}^3$.

The case $g/K \to \infty$ (or the intermediate case $g/K = \text{const}$) cannot be studied by perturbation theory and the asymptotics of $\sigma(\omega; K, g)$ as $g/K \to \infty$ is very sensitive to the behavior of $V(x)$ as $|x| \to \infty$. Let firstly V have a compact support. If $g = c\mathrm{K}^2 \to \infty$, $c = \text{const}$, it is shown in [5] that under certain assumptions (including assumptions on the corresponding classical system)

$$\sigma(\omega\,;\mathrm{K},g) \to 2\sigma_{cl}(\omega), \tag{1.6}$$

where $\sigma_{cl}(\omega)$ is a total classical cross-section for the direction ω of the incident beam of particles. More precisely, in [5] it is proven that (1.6) holds if its left-hand side is averaged over some small energy interval. Note that generically $\sigma_{cl}(\omega)$ does not depend on the energy and $\sigma_{cl}(\omega)$ equals the square of the projection of supp V on the plane Λ_ω, orthogonal to ω. The simpler case $g \to \infty$, $\mathrm{K} \to \infty$, $g \leq c\mathrm{K}^{2-\gamma}$, $\gamma > 0$, was discussed in [6] where the asymptotics (1.6) (without averaging over energy) was justified with the help of the so-called eikonal approximation. In this region one can evaluate also the (logarithmically growing) asymptotics of $\sigma(\omega\,;\mathrm{K},g)$ for exponentially decaying potentials. Outside of the region $g \leq c\mathrm{K}^2$ only upper bounds on $\sigma(\omega\,;\mathrm{K},g)$ are known. Namely, in [7], [8] it is shown that:

$$\int_{1-\varepsilon}^{1+\varepsilon} \sigma(\omega\,;\mathrm{K}s,g)ds \leqslant \mathrm{C}, \qquad \mathrm{K} \geqslant \mathrm{K}_0, \qquad 2\varepsilon < 1, \tag{1.7}$$

where C depends only on the size of the support of V but not on K and g. In [8] the problem was posed to obtain the bound (1.7) without averaging over energy. However, as found in [9] such sharp-energy bound fails in general to be true. Namely, for spherically-symmetric (radial) $\mathrm{V}(x) = \mathrm{V}(r)$, $r = |x|$, with a non-trivial negative part and fixed K, a sequence $g_l = g_l(\mathrm{K}) \to \infty$ was constructed in [9] such that

$$\sigma(\mathrm{K},g_l) \geqslant c(\mathrm{K})g_l^{1/2}. \tag{1.8}$$

The growth of $\sigma(\mathrm{K},g)$ for some sequence g_l has a resonant nature, which is discussed more thoroughly in section 2. On the contrary, for repulsive (not necessary radial) potentials V, $\dfrac{\partial \mathrm{V}}{\partial |x|} \leq 0$, the total cross-section is bounded [9] uniformly in the coupling constant:

$$\sigma(\mathrm{K},g) \leqslant \mathrm{C}(\mathrm{K}). \tag{1.9}$$

This result is improved in section 4 where (1.9) is established for all non negative potentials.

Now we turn to the case of potentials with a power-like behavior at infinity. Under the assumption (1.2) the upper bound

$$\int_{1-\varepsilon}^{1+\varepsilon} \sigma(\omega\,;\mathrm{K}s,g)ds \leqslant \mathrm{C}(g/\mathrm{K})^{\varkappa}, \quad \mathrm{K} \geqslant \mathrm{K}_0 > 0, \quad 2\varepsilon < 1, \qquad g/\mathrm{K} \geqslant c > 0, \quad \varkappa = \varkappa(\alpha) = 2(\alpha-1)^{-1}, \tag{1.10}$$

is proven in [7], [8]. In [10] it was conjectured that as $g/K \to \infty$ the asymptotics of $\sigma(\omega; K, g)$ is determined only by the asymptotics of $V(x)$ as $|x| \to \infty$. Namely, assume that

$$V(x) = |x|^{-\alpha}\Phi(x/_{|x|}) + O(|x|^{-\alpha}), \quad |x| \to \infty. \tag{1.11}$$

The hypothesis of [10] is that

$$\sigma(\omega; K, g) \sim \sigma_0(\omega)(g/2K)^{\varkappa}, \quad K \geqslant K_0 > 0, \quad g/K \to \infty, \tag{1.12}$$

where

$$\sigma_0(\omega) = \pi\,[2\Gamma(\varkappa)\sin(\pi\varkappa/2)]^{-1} \times \int_{\mathbb{S}_\omega} d\psi \left| \int_0^\pi \Phi(\omega\cos\theta + \psi\sin\theta)\sin^{\alpha-2}\theta d\theta \right|^{\varkappa} \tag{1.13}$$

and $\mathbb{S}_\omega$ is a unit circle in the plane Λ_ω. For radial potentials the validity of (1.12), (1.13) was asserted in the book [1] on the basis of the asymptotics of phase shifts $\delta_l(K, g)$ for large l, K and g. By analogy with the radial case the formulae (1.12), (1.13) were formally derived in [10] from the asymptotics of the eigenvalues $\mu_n^{\pm}(K, g)$, $|\mu_n^{\pm}| = 1$, $\pm \operatorname{Im} \mu_n^{\pm} > 0$ of the scattering matrix $S(K, g)$. However in [10] the asymptotics of $\mu_n^{\pm}(K, g)$ as $n \to \infty$ was established for fixed K and g so that the calculations of [10] may be regarded only as heuristic. At present the asymptotics (1.12) for $V(x)$ obeying (1.11) is rigorously proven in case $g/K \to \infty$, $g \leq cK^2$, where $c = c(V)$ is sufficiently small number (and in particular if $g \leq cK^{2-\gamma}$, $\gamma > 0$). This result was reported in [6] and its detailed proof based on the eikonal approximation will be published elsewhere.

In section 3 we give the precise formulation and a sketch of the proof (the details may be found in [11]) of (1.12) for radial potentials. It turns out that for non negative V the conditions of validity of (1.12) are much broader than in general case but the quasi-classical limit is always permitted. We emphasize that our proof of (1.12) does not require any assumptions on the classical system corresponding to (1.1). The proof of (1.12) is based on the analysis of phase shifts $\delta_l(K, g)$ in the region where $l^{\alpha-1}$ is of the same order as $gK^{\alpha-2}$. The technique developped here permits also to find the asymptotics of $\sigma(K, g)$ for potentials with a strong positive singularity $V(r) \sim v_0 r^{-\beta}$, $v_0 > 0$, $\beta > 2$, as $r \to 0$ in the region $g/K \to 0$, $gK^{\beta-2} \to \infty$ (and in particular in the high-energy limit $K \to \infty$, g fixed). Note that for such potentials the right-hand side of (1.5) is infinite so that the formula (1.5) fails certainly to be true. We show that in contrast to regular potentials the asymptotics of $\sigma(K, g)$ is determined only by the singularity of $V(r)$ at $r = 0$ and as $g/K \to 0$ the total cross-section is vanishing slower than in a regular case.

In a final section 4 we prove some sharp-energy upper bounds on $\sigma(K, g)$.

This work is in progress now and we report two results here. Firstly, we show that under assumption (1.2)

$$\sigma(K, g) \leqslant C(g/K)^2 . \tag{1.14}$$

Secondly, for positive potentials with compact support we establish the above-mentioned bound (1.9).

In conclusion of this introduction note that the condition $x \in \mathbb{R}^3$ is in essential and all results can be easily carried over to $\mathbb{R}^m$, $m \geq 2$.

2. ON THE RESONANT SCATTERING BY A NEGATIVE POTENTIAL

Let us firstly give a precise definition of the total scattering cross-section for a radial potential $V(x) = V(r)$, $r = |x|$. Consider a set of equations

$$- y'' + l(l + 1)r^{-2}y + gV(r)y = K^2y , \tag{2.1}$$

describing particles with orbital quantum numbers $l = 0, 1, 2, \ldots$ Assume that $V(r)$ is bounded away from the point $r = 0$, $V(r) = O(r^{-\beta})$, $\beta < 2$, as $r \to 0$ and

$$| V(r) | \leqslant Cr^{-\alpha}, \quad \alpha > 2, \quad r \geqslant r_0 > 0 . \tag{2.2}$$

The equation (2.1) has a real regular solution $\psi_l(r) = \psi_l(r ; K, g)$ satisfying $\psi_l(r) = O(r^{l+1})$, $r \to 0$. As $r \to \infty$

$$\psi_l(r) \sim A_l \sin (Kr - 2^{-1}\pi l + \delta_l), \quad A_l \neq 0 , \tag{2.3}$$

where phase shifts $\delta_l = \delta_l(K, g)$ are determined by (2.3) up to a summand πn, n integer. In terms of phase shifts

$$\sigma(K, g) := 4\pi K^{-2} \sum_{l=0}^{\infty} (2l + 1) \sin^2 \delta_l(K, g) , \tag{2.4}$$

which is consistent with (1.3), (1.4) for a general case. The total cross-section is finite if $\alpha > 2$ but even for potentials with compact supports it is not uniformly bounded as $g \to \infty$.

THEOREM 1. — Let $V(x) = V(r)$ have a compact support and $V(r) < 0$ on a set of a positive Lebesgue measure in $\mathbb{R}_+$. Then for each $K > 0$ there exists a sequence $g_l = g_l(K) \to \infty$ as $l \to \infty$ such that the lower bound (1.8) holds. The constant $C = C(K)$ in (1.8) can be chosen common for all $K \in (0, K_0]$, $K_0 < \infty$.

The proof of this theorem relies on the following:

LEMMA 1. — Under the assumptions of Th. 1 for all sufficiently large l there exists a coupling constant $g_l = g_l(K)$ such that $\delta_l(K, g_l) = \pi/2$ and $C_1 l \leq g_l \leq C_2 l^2$, $C_j > 0$. Constants $C_j = C_j(K)$ may be chosen common for all $K \in (0, K_0]$, $K_0 < \infty$.

Once Lemma 1 is proven, the total cross-section $\sigma(K, g_l)$ can be bounded below by

$$4\pi K^{-2}(2l + 1)\sin^2\delta_l(K, g_l) = 4\pi K^{-2}(2l + 1) \geqslant c(K)g_l^{1/2},$$

which proves Th. 1. The detailed proof of Lemma 1 is given in [9]. Here we note only that the number $g_l(K)$ may be chosen in the following way. Let $V(r) = 0$ for $r \geq \rho$, and let N be the Neumann function. Consider the boundary-value problem

$$-y'' + [l(l+1)r^{-2} - K^2]y = -gV(r)y, \quad r \in (0, \rho), \tag{2.5}$$

$$y(r) = O(r^{l+1}),\ r \to 0,\ \frac{y'(\rho)}{y(\rho)} = \left.\frac{\frac{d}{dr}[r^{1/2}N_{l+1/2}(Kr)]}{r^{1/2}N_{l+1/2}(Kr)}\right|_{r=\rho} \tag{2.6}$$

with g as a spectral parameter. Under assumptions of Th. 1 this problem has a discrete spectrum with $+\infty$ (and possibly $-\infty$ also) as an accumulation point. Let now $g_l(K)$ be the first positive eigenvalue of (2.5), (2.6). Then $g_l(k)$ satisfies all the requirements of Lemma 1. Note that Th. 1 can be easily generalized to potentials with non-compact supports.

Here we discuss the phenomena of the growth of the total cross-section from the physics point of view. To make things transparent assume that $V(r) \leq 0$. For orbital momentum l, $l(l+1) \geq K^2\rho^2$, the effective potential

$$V_{eff}(r) = l(l+1)r^{-2} + gV(r)$$

does not allow a classical particle with an energy K^2 to penetrate into the region $r \leq r_0$ where $r_0 = r_0(l, K) = [l(l+1)]^{1/2}K^{-1}$ is a turning point. Thus for large l a classical particle does not « feel » the potential well $gV(r)$ supported in $r \leq \rho$. The centrifugal term $l(l+1)r^{-2}$ separates this well from the classicaly allowed region by the potential barrier with the height of an order l^2 and the width of an order l. In contrast to a classical, a quantum particle can penetrate through such a barrier on account of tunneling. Thus the potential $gV(r)$ perturbates all phase shifts δ_l but with the growth of the barrier the influence of $gV(r)$ is generically quickly vanishing so that δ_l are small for large l. However, our analysis shows that for the constructed $g_l(K)$ the behavior of a quantum particle in a field $V_{eff}(r)$ is very different from that in a « free » field ($l(l+1)r^{-2}$ if the energy K'^2 is close to K^2. The jump of the phase shift up to $\pi/2$ can be naturally explained by the existence of the quasistationary state in the field V_{eff}. When such a state exists a quantum particle, tunneling through a barrier, is detained in a potential well for a large time (in corresponding quantum units). Since an energy of a particle is positive, a proper bound state does not exist so that a particle tunnels again to infinity contributing to the total cross-section. This ensures the sharp (resonant) peak of $\sigma(K', g_l(K))$ as $K' \to K$. Thereby this peak gets sharper as $l \to \infty$.

In a different situation the described phenomena of the resonant growth of the total cross-section is well-known (Gamow's theory) and is discussed e. g. in the book [12]. In this theory one considers a quantum particle in a deep potential well (due to nuclear forces) which for large r is screened by a repulsive Coulomb potential. In contrast to this problem our potential $gV(r)$ is negative and a positive barrier arises only on account of a centrifugal term by a separation of variables. For negative potentials the existence of resonant peaks of the total cross-section was not, as far as we know, discussed earlier.

3. THE ASYMPTOTICS OF THE TOTAL CROSS-SECTION FOR RADIAL POTENTIALS

The aim of this section is to find the conditions of the validity of the asymptotics (1.12), (1.13) and its rigorous proof for radial potentials $V(x) = V(r)$. The detailed exposition of the results below can be found in [11]. Set again $\varkappa = \varkappa_\alpha = 2(\alpha - 1)^{-1}$ and

$$\chi_\alpha = (4^{-1}\pi^{2\alpha-1})2^{-1}\varkappa_\alpha[\Gamma(\varkappa_\alpha^{-1})\Gamma^{-1}(2^{-1}\alpha)]^{\varkappa_\alpha}[\Gamma(\varkappa_\alpha)\sin(\pi 2^{-1}\varkappa_\alpha)]^{-1}. \quad (3.1)$$

THEOREM 2. — Assume that $V(r) = O(r^{-\beta})$, $\beta < 2$, as $r \to 0$ and

$$V(r) = v_0 r^{-\alpha}(1 + 0(1)), \quad \alpha > 2, \quad r \to \infty. \quad (3.2)$$

Then

$$\sigma(K, g)(g/K)^{-\varkappa_\alpha} \to \chi_\alpha |v_0|^{\varkappa_\alpha} \quad (3.3)$$

as $g/K \to \infty$, $g^{3-\alpha}K^{2(\alpha-2)} \to \infty$. Under the additional assumption $V(r) \geq 0$ the relation (3.3) holds in a broader region $g/K \to \infty, gK^{\alpha-2} \to \infty$.

Let us discuss the assumptions of Th. 2. Though not assumed explicitly, the condition $g \to \infty$ is a consequence of $g/K \to \infty$, $gK^{\alpha-2} \to \infty$. On the contrary, for $\alpha < 3$ and for $V \geq 0$ we permit bounded K and even the case $K \to 0$. Thus for nonnegative potentials the asymptotics (3.3) holds true in a large coupling limit $g \to \infty$, K fixed. In a general case we can assert its validity only for $\alpha \in (2, 3)$. This is connected with the existence of the lower bound (1.8) which shows that (3.3) is certainly destroyed for $\alpha > 5$, when $\varkappa_\alpha < 1/2$. For $\alpha \in [3, 5]$ the validity of (3.3) as $g \to \infty$, K fixed, is an open question. What a quasi-classical limit $g = c\mathrm{K}^2 \to \infty$ is concerned, it is always permitted by the conditions of Th. 2. We emphasize that no assumptions on the corresponding classical system are thereby necessary. Note also that the value (3.1) of the asymptotic coefficient χ_α is consistent with the general formula (1.13).

Our proof of Th. 2 is based on the study in its conditions of the asymptotics of $\delta_l(\mathrm{K}, g)$ for $l^{\alpha-1} \geq dg\mathrm{K}^{\alpha-2}$, $d > 0$ fixed. We remind that by (2.3) the phase shift $\delta_l(\mathrm{K}, g)$ is determined only up to a summand πn, n integer. This ambiguity is standardly eliminated. Namely, $\delta_l(\mathrm{K}, g)$ for fixed g and l may be chosen continuous in K and $\delta_l(\mathrm{K}, g) \to \pi n$ as $\mathrm{K} \to \infty$. Taking $n = 0$ we get the unique phase shift $\delta_l(\mathrm{K}, g)$ which is considered below. Set

$$\tau_\alpha = 2^{-1} \int_1^\infty (s^2 - l)^{-1/2} s^{1-\alpha} ds = 2^{-2}\pi^{1/2}\Gamma(\varkappa_\alpha^{-1})\Gamma^{-1}(\alpha/2).$$

THEOREM 3. — Let V satisfy condition of Th. 2 and let d be any fixed positive number. Then

$$\sup_{l:(l+1/2)^{\alpha-1} \geq dg\mathrm{K}^{\alpha-2}} | \delta_l(g, \mathrm{K})(g\mathrm{K}^{\alpha-2})^{-1}(l + 1/2)^{\alpha-1} + \tau_\alpha v_0 | \to 0 \quad (3.4)$$

as $g/\mathrm{K} \to \infty$, $g^{3-\alpha}\mathrm{K}^{2(\alpha-2)} \to \infty$. Under the additional assumption $\mathrm{V} \geq 0$ (3.4) holds in the region $g/\mathrm{K} \to \infty$, $g\mathrm{K}^{\alpha-2} \to \infty$.

Once Th. 3 is proven the asymptotics (3.3) can be derived from the definition (2.4). Namely, according to (3.4) one can replace asymptotically $\delta_1(\mathrm{K}, g)$ in (2.4) by $-\tau_\alpha v_0 g\mathrm{K}^{\alpha-2}(l + 1/2)^{-\alpha+1}$ and the sum over l by the corresponding integral. Evaluating this integral we arrive at (3.3), (3.1). We do not dwell here upon the details, which can be found in [*11*].

At the heuristic level the asymptotics (3.4) can be deduced from the well-known quasi-classical relation

$$\delta_l(\mathrm{K}, g) \sim \int_{r_l(\mathrm{K},g)}^\infty \{ [\mathrm{K}^2 - l(l+1)r^{-2} - g\mathrm{V}(r)]^{1/2} - [\mathrm{K}^2 - l(l+1)r^{-2}]^{1/2} \} dr, \quad (3.5)$$

where $r_l(\mathrm{K}, g)$ is the largest of roots of two equations $l(l+1)r^{-2} + g\mathrm{V}(r) = \mathrm{K}^2$ and $l(l + 1)r^{-2} = \mathrm{K}^2$. In particular, (3.5) ensures that the asymptotics of $\delta_l(\mathrm{K}, g)$ is determined only by a classically allowed region $r \geq r_l(\mathrm{K}, g)$. The last assertion is easily justified for nonnegative potentials but in the general case it is precisely at this place where the additional restriction $g^{3-\alpha}\mathrm{K}^{2(\alpha-2)} \to \infty$ is required. Formulae (3.5) and hence (3.4) can be most probably justified with the help of the WKB-approximation, what however demands assumptions on the behavior of $\mathrm{V}'(r)$ and $\mathrm{V}''(r)$ at infinity. To avoid these unnatural assumptions we use the so-called variable phase approach (see e. g. [*13*]; note that the variable phase approach was already used in [*8*] to obtain the two-side bounds on $\sigma(\mathrm{K}, g)$ for $\mathrm{V} \geq 0$

and $g \to \infty$, K fixed) which replaces the Schrödinger equation by the first-order nonlinear equation. Namely, let $\nu = \nu_l := l + 1/2$ and $\theta_\nu(\rho) = \theta_\nu(\rho, K, g)$ be the phase shift for the cut-off potential $gV_\rho(r)$, where $V_\rho(r) = V(r)$ for $r \leq \rho$ and $V_\rho(r) = 0$ for $r > \rho$. Then $\theta_\nu(r) = O(r^{2\nu+2-\beta})$ as $r \to 0$ and

$$\lim_{r\to\infty} \theta_\nu(r, K, g) = \delta_{\nu-1/2}(K, g). \tag{3.6}$$

Define now $b_\nu(x) = j_\nu(x)^2 + n_\nu(x)^2$,

$$\zeta_\nu(x) = \int_0^x b_\nu(y)^{-1} dy,$$

where $j_\nu(x) = (2^{-1}\pi x)^{1/2}\mathscr{J}_\nu(x)$, $n_\nu(x) = (2^{-1}\pi x)^{1/2}N_\nu(x)$ and $\mathscr{J}_\nu$, N_ν stand for Bessel and Neumann functions. It can be easily derived from the Schrödinger equation (1.1) that $\theta_\nu(r)$ satisfies the variable phase equation

$$\theta'_\nu(r) = -gK^{-1}V(r)b_\nu(Kr)\sin^2[\theta_\nu(r) + \zeta_\nu(Kr)]. \tag{3.7}$$

It follows from (3.7) that

$$\theta_\nu(r, K, g) \geqslant -\zeta_\nu(Kr) \tag{3.8}$$

and $\theta_\nu \leq 0$ for $V \geq 0$.

Our proof of the asymptotics (3.4) relies on the phase equation (3.7). We describe here only its essential steps. According to (3.6), (3.7)

$$\delta_{\nu-1/2}(K, g) = \theta_\nu(\nu/K, K, g) - Z_\nu(K, g) \tag{3.9}$$

with

$$Z_\nu(K, g) = g\nu K^{-2}\int_1^\infty V(K^{-1}\nu s)b_\nu(\nu s)\sin^2\varphi_\nu(s, K, g)ds \tag{3.10}$$

and

$$\varphi_\nu(s, K, g) = \theta_\nu(K^{-1}\nu s, K, g) + \zeta_\nu(\nu s).$$

By (3.9) the proof of (3.4) is split up into two steps. Firstly we must prove that what the asymptotics of $\delta_{\nu-1/2}(K, g)$ is concerned the summand $\theta_\nu(\nu/K, K, g)$ is insignificant, i. e.

$$\sup_{\nu^{\alpha-1}\geqslant dgK^{\alpha-2}} |\theta_\nu(\nu/K, K, g)|(gK^{\alpha-2})^{-1}\nu^{\alpha-1} \to 0 \tag{3.11}$$

under the assumptions of Th. 3. Essentially, (3.11) means that the classically forbidden region does not contribute to the asymptotics of the phase shifts. The proof of (3.11) is based on the appropriate two-side bounds on $\theta_\nu(r, K, g)$. The lower bound (3.8) is valid irrespective of the sign of V. Combined with $\theta_\nu \leq 0$ its permits easily to prove (3.11) for the case $V \geq 0$.

In the general case the proper upper bound for θ_ν is obtained with the help of the following:

LEMMA 2. — Set

$$\xi_\nu(r) = \int_0^r [(\nu^2 - 1/4)s^{-2} - 1][j'_\nu(s)^2 + n'_\nu(s)^2]^{-1} ds .$$

Assume that for some $r_0 > 0$ and all $r \in (0, r_0)$

$$(\nu^2 - 1/4)r^{-2} + gV(r) - K^2 > 0 . \qquad (3.12)$$

Then for $r \in (0, r_0)$

$$\theta_\nu(r, K, g) < \xi_\nu(Kr) . \qquad (3.13)$$

To deduce (3.11) from (3.8), (3.13) we use well-known [*14*] uniform asymptotic formulae for $\mathcal{J}_\nu(r)$, $\mathcal{J}'_\nu(r)$, $N_\nu(r)$, $N'_\nu(r)$ as $r \to \infty$, $\nu \to \infty$, $r < \nu$. We emphasize that it is just by verifying (3.12) that we need an extra assumption $g^{3-\alpha}K^{2(\alpha-2)} \to \infty$.

The second part of the proof of (3.4) is the evaluation of the asymptotics of the integral (3.10). This can be performed under the assumptions $g/K \to \infty, gK^{\alpha-2} \to \infty$ irrespective of the sign of V. Due to the condition $g/K \to \infty$ we can replace here $V(r)$ by its asymptotics $v_0 r^{-\alpha}$. For $b_\nu(\nu s)$ we use the relation

$$\lim_{\nu \to \infty} b_\nu(\nu s) = s(s^2 - 1)^{-1/2} , \qquad (3.14)$$

which is valid uniformly in s for every compact subinterval of $(1, \infty)$. The relation (3.14) is a consequence of the asymptotics of $\mathcal{J}_\nu(r)$, $N_\nu(r)$ as $r \to \infty$, $\nu \to \infty$, $r > \nu$ (see [*14*]). Thus

$$Z_\nu(K, g) \sim v_0 g K^{\alpha-2} \nu^{1-\alpha} \int_1^\infty (s^2 - 1)^{-1/2} s^{1-\alpha} \sin^2 \varphi_\nu(s, K, g) ds$$

as $g/K \to \infty$, $gK^{\alpha-2} \to \infty$ and $\nu^{\alpha-1} \geq dgK^{\alpha-2}$. Finally we replace here $\sin^2 \varphi_\nu$ by $2^{-1} - 2^{-1}\cos(2\varphi_\nu)$. Integration by parts shows that on account of the phase equation (3.7) the summand with $\cos(2\varphi_\nu)$ does not contribute to the asymptotics (3.4) and therefore

$$Z_\nu(K, g) \sim 2^{-1} v_0 g K^{\alpha-2} \nu^{1-\alpha} \int_1^\infty (s^2 - 1)^{-1/2} s^{1-\alpha} ds .$$

Combining this with (3.9), (3.11) we conclude the proof of Th. 3.

The analysis of phase shifts turns out to be useful also for the study of the high-energy asymptotics of $\sigma(K, g)$ for potentials $V(r)$ with a strong positive singularity at $r = 0$. Assume that $V(r)$ is bounded away from the point $r = 0$ and as $r \to 0$

$$V(r) = v_0 r^{-\beta} + 0(r^{-\beta}),\ v_0 > 0,\ \beta > 2 . \qquad (3.15)$$

The numbers $\varkappa_\beta = 2(\beta - 1)^{-1}$ and χ_β (see (3.1)) are determined now by the singularity of $V(r)$.

THEOREM 4. — Let V satisfy (3.15) as $r \to 0$ and $V(r) = O(r^{-\alpha})$, $\alpha > 2$, as $r \to \infty$. Then

$$\sigma(K, g)(v_0 g/K)^{-\varkappa_\beta} \to \chi_\beta \tag{3.16}$$

as $g/K \to 0$, $gK^{\beta-2} \to \infty$.

Note that under the assumptions of Th. 4 necessarily $K \to \infty$. On the contrary, if $K \to \infty$ the conditions of Th. 4 are fulfilled if $g = \text{const}$ or $g \to \infty$, $g = 0(K)$. The fall-off $g \to 0$ is also permitted though it cannot be too fast because of the condition $gK^{\beta-2} \to \infty$. This is qualitatively different from the conditions of the validity of the Born formula (1.5) in a non-singular case where $g \to 0$ only helps.

For a purely power potential $V(r) = v_0 r^{-\alpha}$, $v_0 > 0$, $\alpha > 2$, the asymptotics (3.3) (or (3.16), what is the same) is true under the unique assumption $gK^{\alpha-2} \to \infty$. The conditions $g/K \to \infty$ or $g/K \to 0$ were used only to replace a potential $V(r)$ by its asymptotics as $r \to \infty$ or $r \to 0$. In conclusion of this section we note that the analysis of phase shifts permits also to find the asymptotics of the forward scattering amplitude under assumptions similar to those of Theorems 2 and 4.

4. UPPER BOUNDS ON THE TOTAL SCATTERING CROSS-SECTION

Let us define firstly the scattering matrix $S(K, g)$ for the Schrödinger equation (1.1) in a non-radial case. We assume here (1.2). Set $X = |V|^{1/2}$, $U = \operatorname{sgn} V$, $H_0 = -\Delta$ and $R_0(z) = (H_0 - z)^{-1}$ in the space $\mathscr{H} = L_2(\mathbb{R}^3)$. Then, as is well-known, the operator function

$$A(z) = XR_0(z)X, \qquad z \in \mathbb{C} \setminus \mathbb{R}_+ ,$$

is analytic in a Hilbert-Schmidt norm $\| \cdot \|_2$ and is continuous in this norm as z approaches the cut over $\mathbb{R}_+$. Moreover, the point -1 does not belong to the spectrum of the operator $gA(K^2 \pm i0)U$, $K > 0$. Define now on $L_2(\mathbb{R}^3) \cap L_1(\mathbb{R}^3)$ the operator Z_K:

$$(Z_K f)(\omega) = 2^{-1/2} K^{1/2} (2\pi)^{-3/2} \int_{\mathbb{R}^3} \exp(-iK\langle \omega, x \rangle) f(x) dx, \ \omega \in \mathbb{S}^2 .$$

Then the operator $Z_K X$ is extended to a compact operator from $\mathscr{H}$ to $\mathscr{M} = L_2(\mathbb{S}^2)$ and

$$2\pi i (Z_K X)^* (Z_K X) = A(K^2 + i0) - A(K^2 - i0), \tag{4.1}$$

which is a usual relation between a spectral measure and boundary values of a resolvent.

Now the scattering matrix $S(K, g)$ can be correctly defined by the equality

$$S(K, g) - I = -2\pi i g(Z_K X)U(I + gA(K^2 + i0)U)^{-1}(Z_K X)^* . \quad (4.2)$$

Note that the right-hand side of (4.2) is a product of bounded operators and hence $S(K, g)$ is a bounded operator in the space $\mathcal{M}$. Moreover, as is well-known (and can be easily seen from (4.1)) the operator $S(K, g)$ is unitary in $\mathcal{M}$. In terms of $S(K, g)$ the averaged total cross-section is defined by (1.4), where the right hand side is finite under the assumption (1.2).

We need also the concept of s-numbers, or singular numbers (see e. g. [*15*]) of a bounded operator A in a Hilbert space $\mathcal{H}$. Let $\mathcal{K}_n$ be a set of all n-dimensional operators. Then by definition

$$s_1(A) = \| A \|, \; s_{n+1}(A) = \min_{L \in \mathcal{K}_n} \| A - L \| . \quad (4.3)$$

Note the inequality

$$s_{n+m-1}(A_1 A_2) \leqslant s_m(A_1) s_n(A_2) . \quad (4.4)$$

For a compact A the singular number $s_n(A)$ is the n^{th} eigenvalue (multiplicities taken into account) of a positive compact operator $(A^*A)^{1/2}$. Since we consider here not only compact A but also operators with compact difference $A - I$, it is convenient to use the more general definition (4.3). Moreover, we need the following lemma which we were unable to find in the literature.

LEMMA 3. — Let A be compact, -1 does not belong to its spectrum and $s_{n+1} \leq \gamma < 1$. Then $s_{n+1}((I + A)^{-1}) \leq (1 - \gamma)^{-1}$.

Proof. — The operator A can be decomposed as $A = K_n + B_n$, where $K_n \in \mathcal{K}_n$ and $\| B_n \| \leq \gamma$. It follows that $I + A = (I + B_n)(I + L_n)$ with $L_n = (I + B_n)^{-1} K_n \in \mathcal{K}_n$. Operators $I + A$ and $I + L_n$ are invertible simultaneously and $(I + L_n)^{-1} = I + M_n$ with $M_n = -L_n(I + L_n)^{-1} \in \mathcal{K}_n$. Thus $(1 + A)^{-1} = (I + M_n)(I + B_n)^{-1}$ and by (4.4)

$$s_{n+1}((I + A)^{-1}) \leqslant s_{n+1}(I + M_n) \| (I + B_n)^{-1} \| \leqslant (1 - \gamma)^{-1}$$

since $s_{n+1}(I + M_n) = 1$ according to (4.3). ■

Now we can prove the bound (1.14). Note that

$$\| A \|_2^2 = \sum_{n=1}^{\infty} s_n^2(A)$$

with A belonging to the Hilbert-Schmidt class iff the right-hand side is finite.

THEOREM 5. — Let the condition (1.2) with $\alpha > 2$ be fulfilled. Then the bound (1.14) holds.

Proof. — Denote by $s_n(K, g)$ the s-numbers of the operator $S(K, g) - I$. Then by definition (1.4)

$$\sigma(K, g) = \pi K^{-2} \sum_{m=1}^{\infty} s_m^2(K, g). \tag{4.5}$$

Recollect that $(-\Delta - K^2 \mp i0)^{-1}$ is an integral operator with a kernel $(4\pi |x - x'|)^{-1} \exp(\pm iK|x - x'|)$ and thus

$$\| A(K^2 \pm i0) \|_2 \leqslant C \tag{4.6}$$

with C independent of K. Let $a_n(K) := s_n(A(K^2 + i0)U)$. The bound (4.6) ensures that

$$a_n(K) \leqslant Cn^{-1/2}. \tag{4.7}$$

Choose now the number n so that $ga_n(K) \leq 1/2$ and consider sums (4.5) over $m < n$ and $m \geq n$ separately. Since $s_m(K, g) \leq 2$ by unitarity of $S(K, g)$ and $n \leq Cg^2$ by (4.7), we have that

$$\sum_{m=1}^{n-1} s_m^2(K, g) \leqslant Cg^2. \tag{4.8}$$

To estimate the sum (4.5) over $m \geq n$ we use the definition (4.2) and the inequality (4.4):

$$\sum_{m=n}^{\infty} s_m^2(K, g) = \sum_{p=1}^{\infty} s_{n+2p-2}^2(K, g) + \sum_{p=1}^{\infty} s_{n+2p-1}^2(K, g) \leqslant$$
$$\leqslant 8\pi^2 g^2 \sum_{p=1}^{\infty} s_p^4(Z_K X) s_n^2([I + gA(K^2 + i0)U]^{-1}).$$

By the choice of n the s-number $s_n(gA(K^2 + i0)U) \leq 1/2$ and thus by Lemma 3

$$s_n([I + gA(K^2 + i0)U]^{-1}) \leqslant 2.$$

It follows now that

$$\sum_{m=n}^{\infty} s_m^2(K, g) \leqslant Cg^2 \sum_{p=1}^{\infty} s_p^4(Z_K X) = Cg^2 \| (Z_K X)^*(Z_K X) \|_2^2.$$

Relations (4.1) and (4.6) ensure that the right-hand side here is bounded by Cg^2. Combining it with (4.8), we conclude the proof. ■

Remark. — The proof of Th. 5 shows that the bound (1.14) is essentially of an abstract nature. Namely, let $\tilde{S}(\lambda)$ be a scattering matrix for some pair of self-adjoint operators H_0, $H = H_0 + V$ (if $H_0 \geq 0$, $\lambda = K^2$ and $\tilde{S}(\lambda) = S(K, 1)$ in our previous notation). Then up to some technical assumptions

$$\| \tilde{S}(\lambda) - I \|_2 \leqslant C \| \, | V |^{1/2} R_0(\lambda + i0) \, | V |^{1/2} \|_2 \tag{4.9}$$

if the right-hand side is finite ; here C is some universal constant. Moreover, the same method applies to prove that

$$\| \tilde{S}(\lambda) - I \|_p \leqslant C_p \| \, | V |^{1/2} R_0(\lambda + i0) \, | V |^{1/2} \|_p, \quad 1 \leqslant p < \infty, \tag{4.10}$$

with $\| A \|_p^p = \sum'_{n=1} s_n^p(A)$. The bound (4.10) can be compared with the Birman-Krein inequality [*16*]

$$\int \| \tilde{S}(\lambda) - I \|_1 d\lambda \leqslant 2\pi \| V \|_1, \tag{4.11}$$

where the integral is taken over the absolutely continuous spectrum of H_0. In contrast to (4.11) the bound (4.10) holds true for a fixed value of a spectral parameter λ (without averaging over λ). The proof of (4.10) requires that λ is not an eigenvalue of H, where $\tilde{S}(\lambda)$ is possibly not properly defined. However, (4.10) holds uniformly in λ as λ approaches the isolated eigenvalue of H.

The bound (1.14) can be considerably improved if we assume faster fall-off of $V(x)$ at infinity. Here we report only one result of this type.

THEOREM 6. — Let $V \geq 0$ and let V have a compact support. Then the bound (1.9), with C(K) depending only on K and a size of a support of V, holds.

Proof. — We start again from the definition (4.2), where $U = I$ now, and use the simple identity

$$g Z_K X [I + g X R_0(K^2 + i0) X]^{-1} X Z_K^* = \\ = (K^2 + 1) Z_K Y_g [I + (K^2 + 1) Y_g R_0(K^2 + i0) Y_g]^{-1} Y_g Z_K^* \tag{4.12}$$

with

$$Y_g^2 = T_g (I + T_g)^{-1}, \; T_g = g (H_0 + I)^{-1/2} V (H_0 + I)^{-1/2} \geq 0. \tag{4.13}$$

Note that the right-hand side of (4.12) has the same structure as its left-hand side with Y_g playing the role of gX. Therefore copying the proof of Th. 5 one can establish that

$$\sigma(K, g) \leqslant C(K) \| Y_g R_0(K^2 + i0) Y_g \|_2^2 . \tag{4.14}$$

So it remains to prove that $\| Y_g R_0(K^2 + i0) Y_g \|_2$ is bounded uniformly in g or according to (4.6), that

$$\| (1 + |x|)^\gamma Y_g \| \leqslant C$$

for some $\gamma > 1$. By the Heinz inequality it is sufficient to prove that

$$\| (1 + |x|)^{2\gamma} T_g (I + T_g)^{-1} \| \leqslant C .$$

Let now $\zeta \in C_0^\infty(\mathbb{R}^3)$ and $\zeta(x) = 1$ on a support of V. By commuting operators of multiplications in coordinate and momentum representations of $\mathscr{H}$ it is easy to prove the boundedness of the operator

$$\Omega := (1 + |x|)^{2\gamma} (H_0 + I)^{-1/2} \zeta(x) (H_0 + I)^{1/2}$$

(for any γ). Now by definition (4.13)

$$(1 + |x|)^{2\gamma} T_g = (1 + |x|)^{2\gamma} g (H_0 + I)^{-1/2} \zeta(x) V (H_0 + I)^{-1/2} = \Omega T_g$$

and therefore

$$\| (1 + |x|)^{2\gamma} T_g (I + T_g)^{-1} \| \leqslant \| \Omega \| \, \| T_g (I + T_g)^{-1} \| \leqslant \| \Omega \|$$

since $T_g \geq 0$. ■

REMARK 1. — Instead of the identity (4.12) by the proof of (4.14) we could have used an abstract bound (4.9) for the pair $(H_0 + I)^{-1}$, $(H_0 + gV + I)^{-1}$ combined with the invariance principle.

REMARK 2. — Th. 1 shows that the condition $V \geq 0$ of Th. 6 cannot be omitted.

Further results on the upper bounds for $\sigma(K, g)$ will be described elsewhere.

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