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On the classical and quantum Coulomb scattering

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Abstract. We develop the scattering theory for the Schrödinger operator with the Coulomb potential in the space of an arbitrary dimension d. In particular, we calculate the scattering matrix and show that its spectrum covers the whole unit circle. We also compute the differential cross section and show that it coincides with the classical Coulomb scattering cross section in the dimension $d = 3$ only.

1. Introduction. Quantum and classical scattering cross sections

Our main goal is to attract attention to the fact that, for Coulomb potential scattering, cross sections in classical and quantum mechanics are the same in the dimension $d = 3$ only. As a prerequisite, this requires a precise definition of the quantum Coulomb cross section $\Sigma_{\rm q}$ for an arbitrary dimension d. We show that stationary and time-dependent definitions of $\Sigma_{\rm q}$ coincide and give an explicit formula for $\Sigma_{\rm q}$.

The paper is organized as follows. In this section we recall definitions of classical $\Sigma_{\rm cl}$ and quantum $\Sigma_{\rm q}$ cross sections. For the Coulomb potential, we compute $\Sigma_{\rm cl}$ and announce the formula (formula (1.1)) for $\Sigma_{\rm q}$. In section 2 we collect necessary information about solutions of the Schrödinger equation with the Coulomb potential for an arbitrary dimension d of the space. In particular, we find an explicit expression for the coefficient (the scattering amplitude) a at the outgoing spherical part of the scattering solution. This yields formula (1.1) for the quantum cross section $\Sigma_{\rm q} = |a|^2$. Time-dependent scattering theory for the Schrödinger operator with a Coulomb potential is developed in sections 3 and 4. We show that the corresponding scattering matrix S is a (singular, in some sense) integral operator and its kernel coincides (up to a usual numerical factor) with the scattering amplitude a. As a by-product of our considerations, we describe the structure of the scattering matrix S and check, in particular, that eigenvalues of S are dense on the unit circle.

1.1.

One of the celebrated results of quantum mechanics is that for the purely Coulomb potential the quantum scattering cross section $\Sigma_{\rm q}(\theta; E)$ coincides with the classical one $\Sigma_{\rm cl}(\theta; E)$ for all scattering angles $\theta \in (0, \pi]$ and all energies $E > 0$. In fact, as shown by Gordon and Mott (see, e.g., [6]), for the potential $\boldsymbol{V}(x) = v|x|^{-1}$, $x \in \mathbb{R}^3$,

$$\Sigma_{\rm q}(\theta; E) = (4E)^{-2} v^2 \sin^{-4}(\theta/2).$$

This is exactly the classical Rutherford formula for $\Sigma_{\rm cl}(\theta; E)$.

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It turns out, however, that the formulae for $\Sigma_q(\theta; E)$ and $\Sigma_{cl}(\theta; E)$ are different if $x \in \mathbb{R}^d$ for $d \neq 3$. Indeed, we show that for any $d \geqslant 2$

$$\Sigma_q(\theta; E) = (2k)^{-d+1}\sigma_d(\alpha)\sin^{-2d+2}(\theta/2) \tag{1.1}$$

where $k = (2mE)^{1/2}\hbar^{-1}$, $\alpha = vm^{1/2}(2E)^{-1/2}\hbar^{-1}$ (m is the mass of a particle) and

$$\sigma_d(\alpha) = \begin{cases} \alpha^2(\alpha^2+1)(\alpha^2+2^2)\ldots(\alpha^2+(d-3)^2/4) & \text{if } d \text{ is odd} \quad (1.2) \\ \alpha\tanh(\pi\alpha)(\alpha^2+1/4)(\alpha^2+3^2/4)\ldots(\alpha^2+(d-3)^2/4) & \text{if } d \text{ is even.} \quad (1.3) \end{cases}$$

In particular, $\sigma_2(\alpha) = \alpha\tanh(\pi\alpha)$. In classical mechanics (see subsection 1.5)

$$\Sigma_{cl}(\theta; E) = (4E)^{-d+1}|v|^{d-1}\sin^{-2d+2}(\theta/2). \tag{1.4}$$

The right-hand sides of (1.1) and (1.4) contain the same function $\sin^{-2d+2}(\theta/2)$ of the scattering angle but the numerical coefficients coincide if and only if $\sigma_d(\alpha) = |\alpha|^{d-1}$. This is true for $d = 3$ only.

Note, however, that $|\alpha|^{-d+1}\sigma_d(\alpha) \to 1$ as $|\alpha| \to \infty$ for any d. Thus, the quantum and classical cross sections coincide in the quasi-classical limit for all dimensions d.

Another specific feature of the Schrödinger operator with the Coulomb potential is the so-called 'accidental' degeneracy of its discrete spectrum (in the case $v < 0$). This means that, except for the first few, the eigenvalues corresponding to different values of the orbital quantum number l are the same. We emphasize that this phenomena holds for all dimensions d.

1.2.

Let us compare quantum and classical cross sections for more general potentials $\boldsymbol{V}(x) = v|x|^{-\rho}, x \in \mathbb{R}^d$. If $\rho \neq 1$, one cannot, of course, hope to obtain an explicit formula for $\Sigma_q(\theta)$. However, we can study $\Sigma_q(\theta)$ and $\Sigma_{cl}(\theta)$ in the limit of small scattering angles and compare their singularities as $\theta \to 0$. It is well known (see, e.g., [5]) that in the classical mechanics, for any $\rho > 0$,

$$\Sigma_{cl}(\theta) = \tau_\rho(|v|/E)\theta^{-(d-1)(1+\rho^{-1})}(1 + O(\theta)) \tag{1.5}$$

where

$$\tau_\rho(g) = \rho^{-1}(\pi^{1/2}\Gamma((1+\rho)/2)\Gamma(\rho/2)^{-1}g)^{(d-1)/\rho}$$

and Γ is the gamma function. As shown in [8], in quantum mechanics the same formula for $\Sigma_q(\theta)$ holds if $\rho \in (0, 1)$. We emphasize that not only powers of θ but also the asymptotic coefficients τ_ρ are the same in classical and quantum mechanics.

On the other hand, the asymptotics of the classical and quantum cross sections are different if $\rho > 1$. In the quantum case $\Sigma_q(\theta)$ behaves as $\theta^{-2d+2\rho}$ if $\rho \in (1, d)$ and hence it grows less rapidly than function (1.5) as $\theta \to 0$. If $\rho > d$, then $\Sigma_q(\theta)$ even has a finite limit as $\theta \to 0$.

The Coulomb potential is intermediary between cases $\rho < 1$ and $\rho > 1$, and the behaviour of scattering cross sections is also intermediary between these cases. Indeed, formulae (1.1) and (1.4) show that for the Coulomb potential both quantum and classical cross sections increase as the same power θ^{-2d+2} of θ for any d but the coefficients at this power are different if $d \neq 3$.

1.3.

Recall that in the short-range case $\boldsymbol{V}(x) = \mathrm{O}(|x|^{-\rho}), \rho > (d+1)/2$, the Schrödinger equation

$$-\Delta\psi + V(x)\psi = k^2\psi \qquad k = (2mE)^{1/2}\hbar^{-1} \qquad V = 2m\hbar^{-2}\boldsymbol{V}$$

has, for every incident direction $\omega_0 \in \mathbb{S}^{d-1}$, solutions with the asymptotics

$$\psi(x, \omega_0, k) = \mathrm{e}^{\mathrm{i}k\langle\omega_0, x\rangle} + a(\omega, \omega_0; k)|x|^{-(d-1)/2}\,\mathrm{e}^{\mathrm{i}k|x|} + o(|x|^{-(d-1)/2}) \qquad \omega = x/|x| \quad (1.6)$$

as $|x| \to \infty$. The coefficient $a(\omega, \omega_0; k)$ at the outgoing spherical wave $|x|^{-(d-1)/2}\,\mathrm{e}^{\mathrm{i}k|x|}$ is called the scattering amplitude. The differential scattering cross section in an angle $\mathrm{d}\omega$ around $\omega \neq \omega_0$ at the energy E is defined as $|a(\omega, \omega_0; k)|^2|\mathrm{d}\omega|$. Abusing the terminology somewhat, we call the function

$$\Sigma_{\mathrm{q}}(\omega, \omega_0; E) = |a(\omega, \omega_0; k)|^2 \qquad (1.7)$$

itself the scattering cross section. Of course, for radial potentials $V(x) = V(|x|)$ the scattering amplitude and cross section depend only on the angle θ between ω and ω_0 (and $k > 0$).

The scattering matrix $S(\lambda), \lambda > 0$, associated with the pair $H_0 = -\Delta, H = -\Delta + V$, is well defined for any $\rho > 1$. It is an integral operator with kernel $s(\omega, \omega'; \lambda)$, which in the case $\rho > (d+1)/2$ is related to the scattering amplitude by the formula

$$s(\omega, \omega'; \lambda) = \delta(\omega - \omega') + (2\pi)^{-(d-1)/2}\mathrm{i}\,\mathrm{e}^{\mathrm{i}\pi(d-3)/4}\lambda^{(d-1)/4}a(\omega, \omega'; \lambda^{1/2}) \qquad (1.8)$$

(δ is the Dirac function). This equality may be accepted for the definition of the scattering amplitude for an arbitrary $\rho > 1$. The function $a(\omega, \omega')$ is regular outside of the diagonal and $a(\omega, \omega') = \mathrm{O}(|\omega - \omega'|^{-d+\rho})$ as $|\omega - \omega'| \to 0$. Thus the leading singularity of the kernel (1.8) at the diagonal is $\delta(\omega - \omega')$. This implies, in particular, that the operator $S(\lambda) - I$ is compact and hence eigenvalues of the unitary operator $S(\lambda)$ may accumulate at the point 1 only.

1.4.

For the Coulomb potential there exist (see section 2) solutions of the equation

$$-\Delta\psi + \gamma|x|^{-1}\psi = k^2\psi \qquad \gamma = v2m\hbar^{-2} \qquad k = (2mE)^{1/2}\hbar^{-1} \qquad (1.9)$$

with asymptotics similar to (1.6) but only outside of a conical neighbourhood of the forward direction $\omega = \omega_0$. Moreover, the plane wave $\mathrm{e}^{\mathrm{i}k\langle\omega_0, x\rangle}$ and the spherical wave $|x|^{-(d-1)/2}\,\mathrm{e}^{\mathrm{i}k|x|}$ are distorted. The coefficient for the distorted spherical wave

$$a(\theta; k) = (2\mathrm{i}k)^{-\delta}\Gamma(\delta + \mathrm{i}\alpha)\Gamma(-\mathrm{i}\alpha)^{-1}\sin^{-d+1-2\mathrm{i}\alpha}(\theta/2) \qquad 2\sin(\theta/2) = |\omega - \omega_0| \quad (1.10)$$

is again called the scattering amplitude. Here and below we use the notation $\alpha = \gamma(2k)^{-1}, \delta = (d-1)/2$. According to formula (1.7), we obtain for the differential cross section expression (1.1), where

$$\sigma_d(\alpha) = |\Gamma(\delta + \mathrm{i}\alpha)\Gamma^{-1}(-\mathrm{i}\alpha)|^2.$$

Equalities (1.2), (1.3) for $\sigma_d(\alpha)$ follow from the usual identities for the gamma function.

Section 3 is devoted to a presentation of scattering theory for the Schrödinger operator $H = -\Delta + \gamma|x|^{-1}$ with the Coulomb potential. To a certain extent this theory is contained in the mathematical folklore but, to our surprise, we have not found all necessary results in the literature. We proceed from the time-dependent formulation of the scattering theory suggested in [2], where modified wave operators $W_\pm$ were introduced. Unfortunately, the proof of completeness of $W_\pm$ and calculation of $W_\pm$ and of the scattering operator $\mathcal{S} = W_+^* W_-$ in terms of solutions of the Schrödinger equation were omitted in [2]. We fill in this gap in section 3.

The structure of the Coulomb scattering matrix corresponding to $\mathcal{S}$ is discussed in section 4. Using results of section 3 we show that $S(\lambda)$ may be considered as an integral operator with kernel

$$s(\omega, \omega'; \lambda) = 2^{i\alpha}\pi^{-\delta}\Gamma(\delta + i\alpha)\Gamma(-i\alpha)^{-1}|\omega - \omega'|^{-d+1-2i\alpha}. \tag{1.11}$$

Note, however, that because of the strong diagonal singularity of the function (1.11) an integral operator with such a kernel should be defined (cf [4]) in some special sense. Comparing (1.10), where $\omega_0 = \omega'$, and (1.11) we see that relation (1.8) between the kernel of the scattering matrix and the scattering amplitude is preserved for $\omega \neq \omega'$. Thus, the stationary and time-dependent definitions of the scattering amplitude coincide.

We emphasize that in the Coulomb case the operator $S(\lambda) - I$ is not compact. In fact, we check that eigenvalues of $S(\lambda)$ are dense on the unit circle.

1.5.

Recall the definition of the scattering cross section in the classical mechanics. Consider a beam of particles of constant energy $E > 0$ sent from infinity in some fixed direction $\omega_0 \in \mathbb{S}^{d-1}$. Suppose that the beam has a uniform density $\boldsymbol{N}$ per unit area of the hyperplane Λ_{ω_0} orthogonal to ω_0. Let $\mathrm{d}N$ be the number of particles which, after interaction with a potential $\boldsymbol{V}(x)$, go to infinity in some solid angle $\mathrm{d}\omega \subset \mathbb{S}^{d-1}$ around a (scattering) direction $\omega \neq \omega_0$. This number referred to the density of the incident beam is, normally, proportional to $|\mathrm{d}\omega|$, that is $\mathrm{d}N/\boldsymbol{N} = \Sigma_{\mathrm{cl}}|\mathrm{d}\omega|$. This quantity is called the differential cross section but we use this term for the function Σ_{cl} itself. A particle in the incident beam is labelled by a vector (the impact parameter) $\boldsymbol{b} \in \Lambda_{\omega_0}$ and its outgoing direction ω is a function of $\boldsymbol{b}$. The classical cross section is completely determined by the function $\omega = \omega(\boldsymbol{b})$.

For spherically symmetric potentials $\boldsymbol{V}(x) = \boldsymbol{V}(|x|)$, the function $\Sigma_{\mathrm{cl}}(\omega, \omega_0)$ depends only on the angle θ between ω and ω_0. Moreover, θ is a function of $b = |\boldsymbol{b}|$ only. Suppose that particles with impact parameters from an interval $(b, b + \mathrm{d}b)$ are scattered at angles from an interval $(\theta, \theta + \mathrm{d}\theta)$. Then the number $\mathrm{d}N/\boldsymbol{N}$ is the volume of the layer in $\mathbb{R}^{d-1}$ between the spheres of radius b and $b + \mathrm{d}b$ so that

$$\Sigma_{\mathrm{cl}}(\theta)|\mathrm{d}\omega| = |\mathbb{S}^{d-2}|b^{d-2}|\mathrm{d}b|. \tag{1.12}$$

Let $\mathrm{d}\omega$ be the band on $\mathbb{S}^{d-1}$ limited by the hyperplanes $\langle x, \omega_0\rangle = \cos\theta$ and $\langle x, \omega_0\rangle = \cos(\theta + \mathrm{d}\theta)$; then $|\mathrm{d}\omega| = |\mathbb{S}^{d-2}|\sin^{d-2}\theta|\mathrm{d}\theta|$. Now it follows from (1.12) that

$$\Sigma_{\mathrm{cl}}(\theta) = \sin^{-d+2}\theta\, b(\theta)^{d-2}|\mathrm{d}b(\theta)/\mathrm{d}\theta|. \tag{1.13}$$

A motion in a central potential is plane so that the function $b = b(\theta)$ is the same for all dimensions d. For the Coulomb potential (see, e.g., [5]) $b(\theta) = (2E)^{-1}|v|\cot(\theta/2)$. Substituting this expression into (1.13), we arrive at formula (1.4).

2. Solutions of the Schrödinger equation

In the particular case $d = 3$ the formulae below are contained in almost any textbook on quantum mechanics (see, e.g., [6]). However, we have not found their proper presentation for an arbitrary dimension.

2.1.

Let us first construct scattering solutions for the Schrödinger equation (1.9). We fix an incident direction ω_0 and seek the wavefunction ψ in the form

$$\psi(x) = \mathrm{e}^{\mathrm{i}k\langle\omega_0,x\rangle} f(r - \langle\omega_0, x\rangle) \qquad r = |x|. \tag{2.1}$$

Substituting this expression into (1.9) we obtain an ordinary differential equation

$$2tf''(t) + (d - 1 - 2\mathrm{i}kt)f'(t) - \gamma f(t) = 0$$

for the function f. Therefore,

$$f(t) = cF(-\mathrm{i}\alpha, \delta, \mathrm{i}kt) \qquad \alpha = \gamma(2k)^{-1} \qquad \delta = (d - 1)/2 \qquad c = \text{constant}$$

where $F(a, b, z)$ is the confluent hypergeometric function satisfying the equation

$$zF''(z) + (b - z)F'(z) - aF(z) = 0. \tag{2.2}$$

We choose the regular solution of (2.2) distinguished by the conditions $F(0) = 1$, $F'(0) = a/b$. We need the asymptotic expansion of $F(a, b, z)$ as $z \to \infty$ along the positive part of the imaginary axis:

$$\Gamma(b)^{-1}F(a, b, z) = \Gamma(b - a)^{-1}(-z)^{-a}(1 + \mathcal{G}_\infty(a, a - b + 1, -z)) \\ +\Gamma(a)^{-1}z^{a-b}\,\mathrm{e}^z(1 + \mathcal{G}_\infty(b - a, 1 - a, z)) \tag{2.3}$$

where $\arg(\pm z) = \pm\pi/2$ and

$$\mathcal{G}_N(a, b, z) = \sum_{p=1}^{N}(p!)^{-1}a(a + 1)\ldots(a + p - 1)b(b + 1)\ldots(b + p - 1)z^{-p}.$$

Setting $c = \Gamma(\delta)^{-1}\Gamma(\delta + \mathrm{i}\alpha)(-\mathrm{i})^{-\mathrm{i}\alpha}$ and using (2.3) for $a = -\mathrm{i}\alpha, b = \delta$, we see that function (2.1) satisfies equation (1.9) and

$$\psi(x) = \exp(\mathrm{i}k\langle\omega_0, x\rangle + \mathrm{i}\alpha\ln(kr(1 - \cos\theta)))(1 + \mathcal{G}_N(-\mathrm{i}\alpha, -\mathrm{i}\alpha - \delta + 1, -\mathrm{i}kr(1 - \cos\theta))) \\ +a(\theta; k)r^{-\delta}\exp(\mathrm{i}kr - \mathrm{i}\alpha\ln(2kr)) + \mathrm{O}(r^{-\delta-1}) \qquad N \geqslant \delta \tag{2.4}$$

as $|x| \to \infty$ in any cone $x_d \leqslant cr, c < 1$ (or $\theta \geqslant \theta_0 > 0$). Here θ is the angle (the scattering angle) between x and ω_0, that is $\cos\theta = \langle x, \omega_0\rangle/r$, and the scattering amplitude $a(\theta; k)$ is defined by equality (1.10).

Compared to asymptotics (1.6) of scattering solutions in the short-range case, relation (2.4) differs in several respects.

(1) A conical neighbourhood of the forward direction $\theta = 0$ is excluded.

(2) The first term on the right-hand side of (2.8), corresponding to the incoming plane wave, contains the phase shift $\alpha\ln(kr(1 - \cos\theta))$ and corrections vanishing as r^{-p}, $1 \leqslant p \leqslant \delta$.

(3) The second term, corresponding to the outgoing spherical wave, contains the phase shift $-\alpha\ln(2kr)$.

It is natural to accept the coefficient $a(\theta; k)$ of the modified spherical wave for the scattering amplitude. Of course, one can add an energy-dependent constant $\Xi(k)$ to the phase of the spherical wave, multiplying $a(\theta; k)$ by $\mathrm{e}^{-\mathrm{i}\Xi(k)}$ at the same time. Apparently there is no preferable unique choice of scattering amplitude but its modulus is intrinsically defined. We emphasize that equality (1.10) for the scattering amplitude gives formula (1.1) for cross section (1.7).

2.2.

For radial potentials 'the variables can be separated' in spherical coordinates. Recall that the Laplace–Beltrami operator $-\Delta_0$ on the unit sphere $\mathbb{S}^{d-1}$ has eigenvalues $l(l+d-2)$, $l = 0, 1, \ldots$. The corresponding eigenspace $\mathfrak{h}_l$ has dimension

$$\nu_l(d) = (2l + d - 2)(l + d - 3)!((d - 2)!\, l!)^{-1}. \tag{2.5}$$

Let $Y_l(\omega)$, $\omega \in \mathbb{S}^{d-1}$, be an arbitrary function from the subspace $\mathfrak{h}_l$ (i.e. Y_l is the spherical function), $x = r\omega$ and $\psi(x) = r^{-\delta}\psi_l(r)Y_l(\omega)$. Then equation (1.9) for $\psi(x)$ reduces to the equation

$$-\psi_l'' + \kappa_l r^{-2}\psi_l + \gamma r^{-1}\psi_l = k^2\psi_l \qquad \kappa_l = (l + \delta - 1/2)^2 - 1/4 \tag{2.6}$$

for $\psi_l(r)$. Making the substitution

$$\psi_l(r, k) = r^q\, \mathrm{e}^{-\mathrm{i}kr} f_l(2\mathrm{i}kr) \qquad q = l + \delta \tag{2.7}$$

we obtain

$$z f_l'' + (2q - z) f_l' - (q - \mathrm{i}\alpha) f_l = 0.$$

This is an equation of the form (2.2) so that f_l is the confluent hypergeometric function. Let us set

$$f_l(z) = c_l F(q - \mathrm{i}\alpha, 2q, z) \qquad \text{with } c_l = \mathrm{i}^l (2\pi)^{-1/2}\Gamma(2l + 2)^{-1}\, \mathrm{e}^{-\pi\alpha/2}|\Gamma(l + \delta + \mathrm{i}\alpha)|. \tag{2.8}$$

Then using asymptotics (2.3) we find that

$$\psi_l(r, k) = \mathrm{i}^l (2/\pi)^{1/2} \sin(kr - \alpha\ln(2kr) - (l + \delta - 1)\pi/2 + \eta_l(k)) + \mathrm{O}(r^{-1}) \qquad r \to \infty \tag{2.9}$$

where the phase shifts

$$\eta_l(k) = \arg\Gamma(l + \delta + \mathrm{i}\alpha) \qquad \alpha = \gamma(2k)^{-1}. \tag{2.10}$$

3. Scattering theory

3.1.

Recall the time-dependent formulation [2] (see also [7]) of the scattering theory for Coulomb potentials. Let $H = -\Delta + \gamma|x|^{-1}$ be the self-adjoint operator in the space $L_2(\mathbb{R}^d)$. In the case $d \geqslant 3$ it is defined on the Sobolev class $\mathsf{H}^2(\mathbb{R}^d)$, that is on the same domain as the operator $H_0 = -\Delta$. In the case $d = 2$ its domain consists of functions u which belong to H^2 outside of any neighbourhood of the point $x = 0$ and admit as $|x| \to 0$ the representation $u(x) = u_0(x) + \gamma u_0(0)|x|$, where $u_0 \in \mathsf{H}^2$. Denote by P the orthogonal projection on the continuous subspace of the operator H (of course, P is the identity operator if $\gamma \geqslant 0$).

Let the free dynamics $U_0(t)$ be defined by the equality $U_0(t) = \Phi^* Z(t)\Phi$, where Φ is the Fourier transform and $Z(t)$ is multiplication by the function $z(|\xi|, t)$ with

$$z(k, t) = \exp(-\mathrm{i}k^2 t - \mathrm{i}\gamma(2k)^{-1}\mathrm{sgn}\, t \ln(4|t|k^2)). \tag{3.1}$$

Then the strong limits

$$W_\pm = s - \lim_{t\to\pm\infty} \exp(\mathrm{i}Ht)U_0(t) \tag{3.2}$$

exist. The modified wave operators $W_\pm$ satisfy the intertwining property $HW_\pm = W_\pm H_0$ and are complete, i.e., $W_\pm W_\pm^* = P$. The scattering operator $\mathcal{S} = W_+^* W_-$ commutes with

H_0 and is unitary. Of course, function $z(k,t)$ may be multiplied by an arbitrary function of k of modulus 1 (not depending on t). As we shall see, the choice (3.1) corresponds to the scattering amplitude (1.10), which is also defined up to a unitary factor only.

The simplest proof of these results relies on separation of variables in spherical coordinates (cf subsection 2.2). Let $\mathfrak{P}_l$ be the orthogonal projection on the subspace $\mathfrak{h}_l$ so that

$$\sum_{l=0}^{\infty}\mathfrak{P}_l = I \qquad \text{and} \qquad -\Delta_0 = \sum_{l=0}^{\infty} l(l+d-2)\mathfrak{P}_l. \tag{3.3}$$

If $Y_{l,m}$ is an arbitrary orthonormal basis in $\mathfrak{h}_l$, then (see [1, vol 2, section 11.4, formula (2)]; there is, however, a misprint in this formula)

$$\sum_{m=1}^{\nu_l(d)} Y_{l,m}(\omega)Y_{l,m}(\omega') = ((d-2)|\mathbb{S}^{d-1}|)^{-1}(2l+d-2)G_l^{(d-2)/2}(\langle\omega,\omega'\rangle) \qquad d \geqslant 3 \tag{3.4}$$

where G_l^p are Gegenbauer polynomials and $|\mathbb{S}^{d-1}| = 2\pi^{d/2}/\Gamma(d/2)$ is the surface of the unit sphere. It follows that $\mathfrak{P}_l$ is an integral operator with kernel (3.4).

Let $K = L_2(\mathbb{R}_+; r^{d-1})$ be the L_2-space with weight r^{d-1} and $\mathfrak{H}_l = K \otimes \mathfrak{h}_l$. To put it differently, $\mathfrak{H}_l \subset L_2(\mathbb{R}^d)$ is the subspace of functions of the form

$$u_l(x) = |x|^{-\delta} g(|x|) Y_l(\hat{x}) \qquad \hat{x} = x/|x| \tag{3.5}$$

where $g \in L_2(\mathbb{R}_+)$ and $Y_l \in \mathfrak{h}_l$. According to the first equality (3.3), $L_2(\mathbb{R}^d) = \bigoplus_{l=0}^{\infty}\mathfrak{H}_l$. Every subspace $\mathfrak{H}_l$ is invariant with respect to the Fourier operator Φ which reduces to the Fourier–Bessel transform on $\mathfrak{H}_l$. More precisely, let J_p be the Bessel function and

$$(\Phi_l g)(k) = \mathrm{i}^{-l} k^{1/2} \int_0^{\infty} J_{l+(d-2)/2}(kr) r^{1/2} g(r)\,\mathrm{d}r.$$

Then for function (3.5)

$$(\Phi u_l)(\xi) = |\xi|^{-\delta}(\Phi_l g)(|\xi|) Y_l(\hat{\xi}) \qquad \hat{\xi} = \xi/|\xi|. \tag{3.6}$$

The operator Φ_l is unitary on $L_2(\mathbb{R}_+)$.

Let $\boldsymbol{z}(t)$ be multiplication by function (3.1) in $L_2(\mathbb{R}_+)$ and $U_0^{(l)}(t) = \Phi_l^* \boldsymbol{z}(t)\Phi_l$ so that

$$(U_0^{(l)}(t) f_0)(r) = \mathrm{i}^l r^{1/2} \int_0^{\infty} k^{1/2} J_{l+(d-2)/2}(kr) z(k,t) \hat{f}_0^{(l)}(k)\,\mathrm{d}k \qquad \hat{f}_0^{(l)} = \Phi_l f_0. \tag{3.7}$$

The subspace $\mathfrak{H}_l$ is invariant with respect to $U_0(t)$ and with respect to the Schrödinger operator with a radial potential. Let $T : L_2(\mathbb{R}_+) \to K$ be a unitary operator defined by $(Tg)(r) = r^{-\delta} g(r)$. It is easy to see that

$$U_0(t) = \bigoplus_{l=0}^{\infty} T U_0^{(l)}(t) T^* \otimes I_l \qquad \text{and} \qquad H = \bigoplus_{l=0}^{\infty} T H^{(l)} T^* \otimes I_l \tag{3.8}$$

where I_l is the identity operator on $\mathfrak{h}_l$ and $H^{(l)} = -\mathrm{d}^2/\mathrm{d}r^2 + \kappa_l r^{-2} + \gamma r^{-1}$. Note that operators $H^{(l)}$ are essentially self-adjoint on the domain $C_0^{\infty}(\mathbb{R}_+)$ if $\kappa > 3/4$. If $\kappa = 3/4$ ($d = 2, l = 1$ or $d = 4, l = 0$), then the domain of $H^{(l)}$ is distinguished by the boundary condition $u(r) = \mathrm{O}(r^{3/2})$ as $r \to 0$. If $\kappa = 0$ ($d = 3, l = 0$), then $H^{(l)}$ is self-adjoint on $\mathsf{H}^2(\mathbb{R}_+)$ with the condition $u(0) = 0$. If $\kappa = -1/4$ ($d = 2, l = 0$), then functions from the domain of $H^{(l)}$ satisfy $u(r) = r^{1/2} + \gamma r^{3/2} + \mathrm{O}(r^{5/2})$ as $r \to 0$.

Suppose that wave operators

$$W_{\pm}^{(l)} = s - \lim_{t\to\pm\infty} \exp(\mathrm{i}H^{(l)} t) U_0^{(l)}(t) \tag{3.9}$$

exist for all l. It follows from (3.8) that limits (3.2) also exist and

$$W_\pm = \bigoplus_{l=0}^{\infty} T W_\pm^{(l)} T^* \otimes I_l \qquad \mathcal{S} = \bigoplus_{l=0}^{\infty} T \mathcal{S}_l T^* \otimes I_l \qquad \mathcal{S}_l = (W_+^{(l)})^* W_-^{(l)}. \tag{3.10}$$

If all wave operators $W_\pm^{(l)}$ are complete, i.e. $W_\pm^{(l)}(W_\pm^{(l)})^* = P_l$ (P_l is the orthogonal projection on the continuous subspace of $H^{(l)}$), then, according to (3.10), the wave operators $W_\pm$ are also complete.

3.2.

Let us check the existence and completeness of operators $W_\pm^{(l)}$. At the same time we shall calculate them in terms of solutions of the Schrödinger equation (2.6). Let functions $\psi_l(r, k)$ be defined by formulae (2.7) and (2.8), where $\alpha = \gamma(2k)^{-1}$, and set

$$(\Psi_l f)(k) = \int_0^\infty \overline{\psi_l(r, k)} f(r)\, \mathrm{d}r \qquad f \in C_0^\infty(\mathbb{R}_+). \tag{3.11}$$

Lemma 3.1. The operators Ψ_l are bounded in the space $L_2(\mathbb{R}_+)$, $\Psi_l \Psi_l^* = I$ (orthogonality of the eigenfunctions ψ_l), $\Psi_l^* \Psi_l = P_l$ (their completeness) and $\Psi_l H^{(l)} = k^2 \Psi_l$ (the intertwining property).

The proof of this assertion is the same as in the short-range case. Its result on the generalized Fourier transform Ψ_l is of the same nature as unitarity of the usual Fourier–Bessel transform. Perhaps this result was not noted in the theory of the confluent hypergeometric function.

Lemma 3.2. If $\mathrm{e}^{\pm \mathrm{i}\eta_l(k)} g(k) = g_0(k)$, then

$$\lim_{t\to\pm\infty} \|\exp(-\mathrm{i}H^{(l)}t)\Psi_l^* g - U_0^{(l)}(t)\Phi_l^* g_0\| = 0. \tag{3.12}$$

We give the proof of this lemma in subsection 3.3.

Since $\Phi_l^*\Phi_l = I_l$, lemma 3.2 implies the existence of wave operators (3.9) and the equality $W_\pm^{(l)}\Phi_l^* = \Psi_l^* \mathrm{e}^{\mp \mathrm{i}\eta_l}$, where η_l is multiplication by $\eta_l(k)$. Now the completeness of $W_\pm^{(l)}$ follows from the equality $\Psi_l^*\Psi_l = P_l$. Let us formulate the results obtained.

Proposition 3.3. Wave operators (3.2) exist, are complete and

$$W_\pm^{(l)} = \Psi_l^* \mathrm{e}^{\mp \mathrm{i}\eta_l} \Phi_l \qquad \mathcal{S}^{(l)} = \Phi_l^* \mathrm{e}^{2\mathrm{i}\eta_l} \Phi_l. \tag{3.13}$$

Corollary 3.4. Wave operators (3.2) exist, are complete and admit the representation (3.10). The scattering operator $\mathcal{S}$ is given by equality (3.10), where $\mathcal{S}^{(l)}$ satisfies (3.13).

3.3. Proof of lemma 3.2

We omit here the index 'l'. It suffices to prove (3.12) for $g_0 \in C_0^\infty(\mathbb{R}_+)$ (or, equivalently, $g \in C_0^\infty(\mathbb{R}_+)$). It follows from (3.11) and the intertwining property that

$$(\exp(-\mathrm{i}Ht)\Psi^* g)(r) = \int_0^\infty \psi(r, k)\, \mathrm{e}^{-\mathrm{i}k^2 t} g(k)\, \mathrm{d}k. \tag{3.14}$$

Let us set $\mu_\pm = \exp(\mp \mathrm{i}(l + \delta - 1)\pi/2)$,

$$(\boldsymbol{U}_\pm(t) g)(r) = \pm \mathrm{i}^l (2/\pi)^{1/2} (2\mathrm{i})^{-1} \mu_\pm \int_0^\infty \mathrm{e}^{\pm \mathrm{i}(kr - \gamma(2k)^{-1}\ln(2kr) + \eta(k))}\, \mathrm{e}^{-\mathrm{i}k^2 t} g(k)\, \mathrm{d}k \tag{3.15}$$

and check first that

$$\lim_{t\to\pm\infty} \|\exp(-\mathrm{i}Ht)\Psi^* g - \boldsymbol{U}_\pm(t)g\| = 0. \tag{3.16}$$

The Riemann–Lebesgue lemma (or integration by parts) shows that, for bounded r, integrals (3.14) or (3.15) tend to zero (quicker than any power of $|t|^{-1}$) as $|t| \to \infty$. By (2.9), the function

$$\exp(-\mathrm{i}Ht)\Psi^* g - (\boldsymbol{U}_+(t) + \boldsymbol{U}_-(t))g \tag{3.17}$$

is bounded by Cr^{-1} for large r uniformly in t. Therefore, the norm of function (3.17) tends to zero as $|t| \to \infty$. Furthermore, using the formula

$$\mathrm{e}^{\mathrm{i}(\pm kr - k^2 t)}\,\mathrm{d}k = -\mathrm{i}(\pm r - 2kt)^{-1}\,\mathrm{d}\,\mathrm{e}^{\mathrm{i}(\pm kr - k^2 t)} \tag{3.18}$$

and integrating by parts in (3.15), we find that the function $(\boldsymbol{U}_\mp(t)g)(r)$ is bounded by $C(r + c|t|)^{-1}(1 + |\ln r|), c > 0$, for $\pm t > 0$. Hence, its norm tends to zero as $t \to \pm\infty$. This proves (3.16).

Quite similarly, using representation (3.7) and replacing the Bessel function by its asymptotics as $r \to \infty$ we obtain

$$\lim_{t\to\pm\infty} \|U_0(t)\Phi^* g_0 - \boldsymbol{U}_\pm^{(0)}(t)g_0\| = 0$$

where

$$(\boldsymbol{U}_\pm^{(0)}(t)g_0)(r) = \pm\mathrm{i}^l(2/\pi)^{1/2}(2\mathrm{i})^{-1}\mu_\pm \int_0^\infty \mathrm{e}^{\pm\mathrm{i}(kr - \gamma(2k)^{-1}\ln(4k^2|t|))}\,\mathrm{e}^{-\mathrm{i}k^2 t} g_0(k)\,\mathrm{d}k. \tag{3.19}$$

Thus, for the proof of (3.12) it remains to check that the function

$$\boldsymbol{U}_\pm(t)g - \boldsymbol{U}_\pm^{(0)}(t)g_0 \qquad \mathrm{e}^{\pm\mathrm{i}\eta}g = g_0 \tag{3.20}$$

tends to zero in $L_2(\mathbb{R}_+)$ as $t \to \pm\infty$. Let us compare representations (3.15) and (3.19), and integrate by parts using equality (3.18). The crucial point is that the singularity of $(r - 2k|t|)^{-1}$ is compensated by the vanishing of the function

$$\mathrm{e}^{\mp\mathrm{i}\gamma(2k)^{-1}\ln(2kr)} - \mathrm{e}^{\mp\mathrm{i}\gamma(2k)^{-1}\ln(4k^2|t|)}$$

at the point $r = 2k|t|$. This implies that the norm of function (3.20) is bounded by $|t|^{-1/2}\ln|t|$.

4. The scattering matrix

4.1.

To define the scattering matrix we consider a diagonal representation of H_0. Set $(Yg)(\lambda;\omega) = 2^{-1/2}\lambda^{(d-2)/4}g(\lambda^{1/2}\omega)$. Then $F = Y\Phi : L_2(\mathbb{R}^d) \to L_2(\mathbb{R}_+; L_2(\mathbb{S}^{d-1}))$ is a unitary operator and FH_0F^* acts as multiplication by λ. Since the scattering operator $\mathcal{S}$ commutes with H_0, the operator $F\mathcal{S}F^*$ acts in the space $L_2(\mathbb{R}_+; L_2(\mathbb{S}^{d-1}))$ as multiplication by an operator function $S(\lambda) : L_2(\mathbb{S}^{d-1}) \to L_2(\mathbb{S}^{d-1}), \lambda > 0$, called the scattering matrix.

To calculate the scattering matrix note that, according to (3.6), (3.10) and (3.13),

$$\Phi\mathcal{S}\Phi^* = \bigoplus_{l=0}^{\infty} \mathrm{e}^{2\mathrm{i}\eta_l} \otimes I_l \tag{4.1}$$

where η_l is multiplication by function (2.10). Equality (4.1) can be rewritten in terms of the scattering matrix. Recall that $\alpha = 2^{-1}\gamma\lambda^{-1/2}$.

Lemma 4.1. Let $\mathfrak{P}_l$ be the integral operator with kernel (3.4). Then

$$S(\lambda) = \sum_{l=0}^{\infty} S^{(l)}(\lambda)\mathfrak{P}_l \qquad \text{where} \qquad S^{(l)}(\lambda) = \exp(2\mathrm{i}\eta_l(\lambda^{1/2})) = \frac{\Gamma(l+\delta+\mathrm{i}\alpha)}{\Gamma(l+\delta-\mathrm{i}\alpha)}. \tag{4.2}$$

Thus, the spectrum of the unitary operator $S(\lambda)$ consists of eigenvalues $S^{(l)}(\lambda)$ of multiplicity (2.5). By the Stirling formula,

$$S^{(l)}(\lambda) = \exp(2\mathrm{i}\alpha \ln(l+\delta))(1+\mathrm{O}(l^{-1})) \qquad \text{as} \qquad l \to \infty.$$

Since the function $f(x) = \ln(x+\delta) \to \infty$ but $f'(x) = (x+\delta)^{-1} \to 0$ as $x \to \infty$, this implies.

Proposition 4.2. For any $\lambda > 0$ the eigenvalues of the scattering matrix $S(\lambda)$ are dense on the unit circle.

This is completely different from the short-range case when eigenvalues of the scattering matrix accumulate at the point 1 only (the phase shifts $\eta_l(\lambda)$ tend to zero as $l \to \infty$).

4.2.

Let us now construct the scattering matrix $S(\lambda)$ as an integral operator. One can proceed from expression (4.2) but avoid an apparently difficult problem of summation of this series. To that end, we obtain an expression for the kernel $s(\omega, \omega'; \lambda)$ of $S(\lambda)$ by some heuristic arguments and then check that such an operator $S(\lambda)$ satisfies (4.2). First, by an analogy with the short-range case we assume that $s(\omega, \omega'; \lambda)$ is related to the scattering amplitude $a(\omega, \omega'; k)$ for $\omega \neq \omega'$ by formula (1.8). Since a satisfies (1.10), this gives expression (1.11) for $s(\omega, \omega'; \lambda)$. Second, according to proposition 4.2, the spectral point 1 is exceptional for $S(\lambda)$ in the short-range but not in the Coulomb case. Therefore, it is natural to expect that the Dirac function is dropped out of $s(\omega, \omega'; \lambda)$. Thus we suppose that the scattering matrix $S(\lambda)$ is given by the equality

$$(S(\lambda)f)(\omega) = 2^{2\mathrm{i}\alpha}\pi^{-\delta}\frac{\Gamma(\delta+\mathrm{i}\alpha)}{\Gamma(-\mathrm{i}\alpha)}\int_{\mathbb{S}^{d-1}} |\omega-\omega'|^{-d+1-2\mathrm{i}\alpha} f(\omega')\,\mathrm{d}\omega'. \tag{4.3}$$

One must be careful with a precise definition of this integral operator since its kernel is not integrable in a neighbourhood of the diagonal $\omega = \omega'$. One of the possibilities is to replace $-\mathrm{i}\alpha$ by $-\mathrm{i}\alpha + \varepsilon$, $\varepsilon > 0$, in (4.3) and approximate $S(\lambda)$ by compact operators $S_\varepsilon(\lambda)$ with kernels

$$s_\varepsilon(\omega, \omega'; \lambda) = 2^{2\mathrm{i}\alpha-2\varepsilon}\pi^{-\delta}\Gamma(\delta+\mathrm{i}\alpha-\varepsilon)\Gamma(-\mathrm{i}\alpha+\varepsilon)^{-1}|\omega-\omega'|^{-d+1-2\mathrm{i}\alpha+2\varepsilon}. \tag{4.4}$$

This is similar to the definition proposed in [4].

Let us decompose $S_\varepsilon(\lambda)$ into an orthogonal sum of projectors $\mathfrak{P}_l$.

Lemma 4.3. For any $\varepsilon > 0$

$$S_\varepsilon(\lambda) = \sum_{l=0}^{\infty} S_\varepsilon^{(l)}(\lambda)\mathfrak{P}_l \qquad \text{where} \qquad S_\varepsilon^{(l)}(\lambda) = \frac{\Gamma(l+\delta+\mathrm{i}\alpha-\varepsilon)}{\Gamma(l+\delta-\mathrm{i}\alpha+\varepsilon)}. \tag{4.5}$$

The proof of this lemma is given in subsection 4.4.

Comparing lemmas 4.1 and 4.3, we see that $S(\lambda)$ may be approximated by operators $S_\varepsilon(\lambda)$ in the strong operator sense.

Proposition 4.4. The scattering matrix $S(\lambda)$ satisfies the relation

$$S(\lambda) = s - \lim_{\varepsilon\to 0} S_\varepsilon(\lambda). \tag{4.6}$$

Formulae (4.4) and (4.6) give precise sense to equality (4.3).

4.3.

According to (4.3), the kernel of the scattering matrix $S(\lambda)$ is a smooth function outside of the diagonal $\omega = \omega'$. Its modulus has a singularity $|\omega - \omega'|^{-d+1}$ at the diagonal which is typical (the power $d-1$ equals the dimension of $\mathbb{S}^{d-1}$) for singular integral operators. However, $S(\lambda)$ is an operator from an essentially different class. In fact, it is bounded (and even unitary) due to oscillations $|\omega - \omega'|^{-2\mathrm{i}\alpha}$ which compensate the singularity of its modulus whereas a singular integral operator is bounded because some average value of its kernel is zero.

The structure of $S(\lambda)$ becomes more transparent if one treats it as a pseudo-differential operator. Its principal symbol $p(\omega, b)$ is defined for $\omega \in \mathbb{S}^{d-1}$, $\langle b, \omega\rangle = 0$ (the cotangent bundle of $\mathbb{S}^{d-1}$) and, roughly speaking, it is the Fourier transform of $s(\omega, \omega')$ in the variable $\xi = \omega - \omega'$:

$$p(\omega, b) = \int_{\mathbb{S}^{d-1}} s(\omega, \omega')\, \mathrm{e}^{-\mathrm{i}\langle \omega-\omega', b\rangle}\, \mathrm{d}\omega'.$$

By calculation of the principal symbol we can replace $\mathbb{S}^{d-1}$ by its tangent plane at the point $\omega = \omega'$ and the kernel $s(\omega, \omega')$ by its singularity at $\omega = \omega'$. For spherically symmetric potentials $p(\omega, b)$ depends on $|b|$ only. In particular for kernel (1.11), calculating the Fourier transform in $\mathbb{R}^{d-1}$ (in the sense of distributions) of the function $|\xi|^{-d+1-2\mathrm{i}\alpha}$ we find that $p(\omega, b) = |b|^{2\mathrm{i}\alpha}$. This is an oscillating function as $|b| \to \infty$, whereas in the short-range case it converges to 1 (the Fourier transform of the Dirac function). In this sense the Dirac function disappears from the kernel of the Coulomb scattering matrix.

4.4. Proof of lemma 4.3

Let us take into account the fact that $|\omega - \omega'| = 2\sin(\theta/2)$ and expand (see e.g. [1, vol 2, ch 10]) function (4.4) on the interval $(0, \pi)$ in a series of Gegenbauer polynomials:

$$\sin^{-d+1-2\mathrm{i}\alpha+2\varepsilon}(\theta/2) = \sum_{l=0}^{\infty} B_l A_l^{-1} G_l^{(d-2)/2}(\cos\theta) \qquad d \geqslant 3 \tag{4.7}$$

where

$$A_l = \int_0^\pi (G_l^{(d-2)/2}(\cos\theta))^2 \sin^{d-2}\theta\, \mathrm{d}\theta$$

$$B_l = \int_0^\pi \sin^{-d+1-2\mathrm{i}\alpha+2\varepsilon}(\theta/2) G_l^{(d-2)/2}(\cos\theta) \sin^{d-2}\theta\, \mathrm{d}\theta.$$

Note that

$$(2l + d - 2)2^{d-4} l! A_l = \pi\Gamma(l + d - 2)\Gamma((d-2)/2)^{-2}$$

(see [1, vol 2, section 11.1, formula (26)]) and

$$B_l = \frac{2^{d-2}(-1)^l (d + l - 3)!\Gamma(\delta)\Gamma(-\mathrm{i}\alpha + \varepsilon)\Gamma(1 - \delta - \mathrm{i}\alpha + \varepsilon)}{l!(d-3)!\Gamma(1 - \delta - \mathrm{i}\alpha + \varepsilon - l)\Gamma(\delta - \mathrm{i}\alpha + \varepsilon + l)}$$

(the last equality can be easily deduced from formula 7.311(3) of [3]). Using well known identities for the gamma function we see that

$$2^{-d+1}\pi^{-\delta}\frac{\Gamma(\delta+\mathrm{i}\alpha-\varepsilon)}{\Gamma(-\mathrm{i}\alpha+\varepsilon)}\frac{B_l}{A_l}=\frac{2l+d-2}{(d-2)|\mathbb{S}^{d-1}|}\frac{\Gamma(l+\delta+\mathrm{i}\alpha-\varepsilon)}{\Gamma(l+\delta-\mathrm{i}\alpha+\varepsilon)}.$$

Now (4.5) follows from (4.4), (4.7) and expression (3.4) for the kernel of the projector $\mathfrak{P}_l$.

In the case $d=2$, calculations are much simpler because the role of (4.7) is played by the formula

$$\sin^{-1-2\mathrm{i}\alpha+2\varepsilon}(\theta/2)=f_0+2\sum_{l=1}^{\infty}f_l\cos(l\theta)=\sum_{l=-\infty}^{\infty}f_l\,\mathrm{e}^{\mathrm{i}l\varphi}\,\mathrm{e}^{-\mathrm{i}l\varphi'}$$

where $\omega=(\cos\varphi,\sin\varphi)$, $\omega'=(\cos\varphi',\sin\varphi')$, $\theta=|\varphi-\varphi'|$ and

$$\pi f_l=\int_0^{\pi}\sin^{-1-2\mathrm{i}\alpha+2\varepsilon}(\theta/2)\cos(l\theta)\,\mathrm{d}\theta.$$

Using [1, vol 1, section 1.5.1, formula (30)], we find that

$$f_l=\pi^{-1/2}\frac{\Gamma(-\mathrm{i}\alpha+\varepsilon)}{\Gamma(1/2+\mathrm{i}\alpha-\varepsilon)}\frac{\Gamma(l+1/2+\mathrm{i}\alpha-\varepsilon)}{\Gamma(l+1/2-\mathrm{i}\alpha+\varepsilon)}.$$

This gives again (4.5) with $\delta=1/2$.

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