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A note on the transport cross section

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Abstract
We present a neat formula for the *transport cross section* for spherically symmetric potentials. The formula is the analogy of a well-known expression for the total cross section in terms of phase shifts. For a hard sphere we calculate the *transport cross section* explicitly, which shows that for all positive wavenumbers k, most scattering is in the forward direction.

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Dedicated to R A Minlos on the occasion of his 75th birthday

1. Definition of the transport cross section

First, we define the classical resistance of a body. Let a heavy body be given as a subset $\Omega \subset \mathbb{R}^3$ and consider a flow of particles with mass m in the positive direction of the z-axis (denote the unit vector as $\mathbf{e} = (0, 0, 1)$ with velocity $\mathbf{v} = v\mathbf{e}$). The particles move freely, then undergo several elastic collisions with Ω and finally move freely again with velocity $v\mathbf{e}^+(x)$ where $x \in \mathbb{R}^2$ marks their initial coordinates in $v^\perp$, the plane perpendicular to $\mathbf{v}$. The classical (vector-valued) resistance $\mathbf{R}_{\text{cl}}$ is defined through the formula

$$\mathbf{R}_{\text{cl}}(\Omega) = \int_{v^\perp} (\mathbf{e} - \mathbf{e}^+(x))\, \mathrm{d}x.$$

If the body Ω is axially symmetric (around the z-axis), then $\mathbf{R}_{\text{cl}}$ lies along the z-axis. Since we always assume this to be the case, we define the scalar

$$R_{\text{cl}}(\Omega) = \mathbf{e} \cdot \mathbf{R}_{\text{cl}}(\Omega).$$

When multiplied by mv and by the number of incoming particles per unit area, $\mathbf{R}_{\text{cl}}$ equals the total momentum transferred to Ω. At this point one can ask some interesting questions; already Newton posed and solved the problem of minimizing R_{cl} in the class of axially symmetric convex bodies inscribed in a fixed cylinder. Recently this problem has received renewed attention [3, 7, 11].

We will consider the quantum analogue of R_{cl}, the so-called *transport cross section* (TCS), also called *momentum-transfer cross section*. Minimizing TCS with fixed total *cross section* (CS), as would be the analogue of the classical Newton problem, is clearly far beyond our possibilities, since for calculating TCS we have only some estimates [8] in the Born approximation. In this paper we present an appealing formula for TCS in terms of phase shifts. It is analogous to the well-known formula for CS. As an illustration, we apply this formula in the case of a hard sphere.

Consider a quantum particle with wave vector $\mathbf{k} \equiv k\mathbf{e}$ incident on the body Ω with associated potential

$$V_\Omega(x) = \begin{cases} 0 & \text{if } x \notin \Omega, \\ +\infty & \text{if } x \in \Omega. \end{cases} \tag{1}$$

Basic scattering theory teaches us that the wavefunction Ψ should satisfy the following conditions: the Helmholtz equation:

$$-\Delta\Psi = k^2\Psi, \tag{2}$$

the boundary condition:

$$\Psi|_{\partial\Omega} \equiv 0 \tag{3}$$

and the Sommerfeld radiation criterion (let $\mathbf{q} \equiv \frac{\mathbf{r}}{|\mathbf{r}|} \in S^2$):

$$\Psi = \mathrm{e}^{\mathrm{i}kz} + \frac{f(\mathbf{q})}{|\mathbf{r}|}\,\mathrm{e}^{\mathrm{i}k|\mathbf{r}|} \qquad |\mathbf{r}| \to +\infty. \tag{4}$$

The function $f(\mathbf{q}) = f_\Omega(\mathbf{q}, k)$ goes by the name of *scattering amplitude*. Now we can introduce the quantum TCS:

$$\sigma_T = \frac{1}{k}\int_{S^2} \mathbf{k}\cdot(\mathbf{e}-\mathbf{q})|f(\mathbf{q})|^2\mathrm{d}\mathbf{q}, \tag{5}$$

which yields the classical resistance if we substitute, with $J(F^{-1}(\cdot))$ being the Jacobian of the map F^{-1},

$$|f(\mathbf{q})|^2 = |f_{\mathrm{cl}}(\mathbf{q})|^2 = |J(F^{-1}(\mathbf{q}))| \qquad F : \mathbb{R}^2 \to S^2 : x \to \mathbf{e}^+(x). \tag{6}$$

In the classical case, R_{cl} depends solely on geometrical properties of Ω. In contrast, σ_T depends in a non-trivial way on the wavenumber k.

A quantity which is very well documented in both the quantum and the classical case is the total *cross section* (CS):

$$\sigma = \int_{S^2} |f(\mathbf{q})|^2\,\mathrm{d}\mathbf{q}. \tag{7}$$

In the classical case, one can view σ as measuring the number of particles colliding with the target. In the quantum case, this interpretation of course breaks down (every incoming particle interacts with the target), but it remains true that σ measures the intensity loss of the incident beam. In general, σ depends on the wavenumber k, as shown in figure 1 for the hard sphere, see [1].

Remark that both R_{cl} and σ_T have the dimensions of an *area*, just like the CS σ. It is quite natural to replace the rigid body Ω by a general potential $V(\mathbf{r})$. This means that one has to replace (2), (3) with the stationary Schrödinger equation:

$$-\Delta\Psi + V\Psi = k^2\Psi, \tag{8}$$

which reduces to (2) for V as in (1). Expressions (5) and (7) are still meaningful for general potentials $V(\mathbf{r})$.

2. Result

We restrict ourselves to the class of spherically symmetric potentials $V(\mathbf{r}) = V(|\mathbf{r}|)$. Recall that for these potentials $f(\mathbf{q}) = f(\theta(\mathbf{q}))$ where $\theta \in [0, \pi]$ is defined by

$$\cos\theta = \mathbf{e}\cdot\mathbf{q} \tag{9}$$

Theorem 1. *Let the potential $V(|\mathbf{r}|)$ be such that the scattering amplitude can be expressed as*

$$f(\theta) = \frac{1}{2\mathrm{i}k}\sum_{l=0}^{\infty}(2l+1)(\mathrm{e}^{2\mathrm{i}\delta_l}-1)P_l(\cos\theta), \tag{10}$$

where P_l are the Legendre polynomials, and $\delta_l, l = 0, 1, \ldots,$ are (k-dependent) numbers, called the phase shifts [5].

Then, we have

$$\sigma_T = \frac{4\pi}{k^2}\sum_{l=1}^{\infty} l\cdot\sin^2(\delta_l - \delta_{l-1}). \tag{11}$$

Remark 1. In the mathematical literature, one defines the Rolnik class of potentials V, see [12, vol 2]. For this class one can rigorously prove expansion (10). In the physical literature, one usually says that this expansion is generally valid for potentials falling off faster than the Coulomb potential.

The formula for σ_T should be compared to the well-known formula for the total *cross section* CR:

$$\sigma = \frac{4\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)\sin^2\delta_l.$$

In the case of Ω being the hard sphere with radius r, the solution to (2)–(4) is explicitly known, see e.g. [6]:

$$\tan\delta_l = \frac{j_l(kr)}{n_l(kr)}, \qquad l \geqslant 0,$$

where j_l, n_l are respectively the spherical Bessel and the spherical Hankel functions. Plugging this expression for δ_l in formula (11) and using $\sin^2\delta_l = j_l^2(kr)/\big(j_l^2(kr) + n_l^2(kr)\big)$ and $\cos^2\delta_l = n_l^2(kr)\big/\big(j_l^2(kr) + n_l^2(kr)\big)$, we obtain

$$\sigma_T = \frac{4\pi}{k^2}\sum_{l=1}^{\infty} l\,\frac{(j_l(kr)n_{l-1}(kr) - j_{l-1}(kr)n_l(kr))^2}{\big(j_{l-1}^2(kr) + n_{l-1}^2(kr)\big)\big(j_l^2(kr) + n_l^2(kr)\big)}.$$

In figure 1, the dependence of respectively the CS and the TCS (both classical and quantum) on the velocity k is shown. It is well known (i.e. [6]) that in the high-energy limit, the quantum CS is twice the classical CS. Remark that however the quantum TCS and classical resistance are equal in this limit. We see from the graph that for $k = 0$, we have $\sigma_T = \sigma$. Indeed, at low energies, one has isotropic scattering. For positive k, the scattering is anisotropic and in fact we have for all positive k, $\sigma_T < \sigma$, or, in other words

$$\int_{S^2}\cos\theta|f(\mathbf{q})|^2\,\mathrm{d}\mathbf{q} > 0, \qquad \cos\theta = \mathbf{e}\cdot\mathbf{q},$$

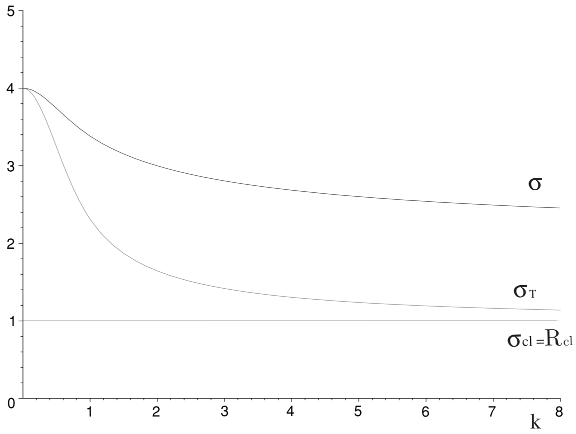

Figure 1. Transport cross section σ_T and classical resistance R_{cl}; total cross section σ and classical total cross section σ_{cl} for the hard sphere with radius $r = \pi^{-1/2}$.

which shows that there is more forward scattering than backscattering. The question to what extent this is a general feature will be addressed in [4]. In fact, for smooth enough bodies Ω, the correct high-energy behaviour [9, 4] of $f(\mathbf{q})$ is given by (in the sense of distributions)

$$\lim_{k\to+\infty} |f|^2 = |f_{\mathrm{cl}}|^2 + \sigma_{\mathrm{cl}}\delta_{\mathbf{e}}, \tag{12}$$

where $\delta_{\mathbf{e}}$ is the Dirac delta distribution on the sphere, concentrated in $\mathbf{e}$, f_{cl} is the classical scattering amplitude given in (6) and σ_{cl} is the total CS calculated from f_{cl}. From formula (12), one can immediately deduce that

$$\lim_{k\to+\infty} \sigma = 2\sigma_{\mathrm{cl}}, \qquad \lim_{k\to+\infty} \sigma_T = R_{\mathrm{cl}}.$$

3. Proof of theorem 1

We start from expression (10) and calculate

$$\sigma_T - \sigma = -2\pi \int_{-1}^{1} \mathrm{d}\cos\theta |f(\theta)|^2 \cos\theta. \tag{13}$$

Using the recursion relation $xP_n(x) = \frac{n+1}{2n+1}P_{n+1}(x) + \frac{n}{2n+1}P_{n-1}(x)$ and the orthogonality of the Legendre polynomials, we obtain that (13) equals

$$\frac{-2\pi}{4k^2}\int_{-1}^{1}\mathrm{d}\cos\theta\sum_{n=1}^{\infty}\cos\theta P_n(\cos\theta)P_{n-1}(\cos\theta)(2n+1)(2n-1)a_{n,n-1}, \tag{14}$$

where

$$\begin{aligned} a_{n,n-1} &= (\mathrm{e}^{2\mathrm{i}\delta_n} - 1)(\mathrm{e}^{-2\mathrm{i}\delta_{n-1}} - 1) + (\mathrm{e}^{-2\mathrm{i}\delta_n} - 1)(\mathrm{e}^{2\mathrm{i}\delta_{n-1}} - 1) \\ &= 2(\cos 2(\delta_n - \delta_{n-1}) - \cos 2\delta_n - \cos 2\delta_{n-1} + 1) \\ &= 4(-\sin^2(\delta_n - \delta_{n-1}) + \sin^2\delta_n + \sin^2\delta_{n-1}). \end{aligned} \tag{15}$$

(14) equals

$$-\frac{\pi}{2k^2}\sum_{n=1}^{\infty}\frac{n}{2n+1}\|P_{n-1}\|^2_{L_2[0,1]}(2n+1)(2n-1)a_{n,n-1}. \tag{16}$$

Using the normalization $\|P_{n-1}\|_{L_2[0,1]} = \frac{2}{2n-1}$, we obtain that (16) equals

$$-\frac{\pi}{2k^2}\sum_{n=1}^{\infty}\frac{n}{2n+1}\frac{2}{2n-1}(2n+1)(2n-1)a_{n,n-1} = -\frac{\pi}{k^2}\sum_{n=1}^{\infty} n a_{n,n-1}$$
$$= \frac{4\pi}{k^2}\sum_{n=1}^{\infty} n\sin^2(\delta_n - \delta_{n-1}) - \frac{4\pi}{k^2}\sum_{n=1}^{\infty} n\sin^2\delta_n - \frac{4\pi}{k^2}\sum_{n=1}^{\infty} n\sin^2\delta_{n-1}. \qquad (17)$$

And we finally have

$$\sigma_T - \sigma = \frac{4\pi}{k^2}\sum_{n=1}^{\infty} n\sin^2(\delta_n - \delta_{n-1}) - \sigma \qquad (18)$$

because

$$\frac{4\pi}{k^2}\left(\sum_{n=1}^{\infty} n\sin^2\delta_n + \sum_{n=1}^{\infty} n\sin^2\delta_{n-1}\right) = \frac{4\pi}{k^2}\left(\sum_{n=0}^{\infty} n\sin^2\delta_n + \sum_{n=0}^{\infty}(n+1)\sin^2\delta_n\right)$$
$$= \frac{4\pi}{k^2}\sum_{n=0}^{\infty}(2n+1)\sin^2\delta_n = \sigma.$$

theorem 1 is proven.

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