ANNALES DE L'INSTITUT FOURIER

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Annales de l'institut Fourier, tome 25, nº 3-4 (1975), p. 317-321
<http://www.numdam.org/item?id=AIF_1975__25_3-4_317_0>

Ann. Inst. Fourier, Grenoble
25, 3 et 4 (1975), 317-321.

SCATTERING LENGTH AND CAPACITY

by M. KAC (1) and J.-M. LUTTINGER (2)

Dédié à Monsieur M. Brelot à l'occasion de son 70e anniversaire.

1. Let $q(\vec{R}) \geqslant 0$ ($\vec{R}$ a three-dimensional vector) and

$$\int q(\vec{R})\, d\vec{R} < \infty \tag{1.1}$$

the integration being extended over the whole three-dimensional Euclidean space E^3.

The scattering problem consists in finding the solutions of the Schroedinger equation

$$\frac{1}{2} \nabla^2\Phi - q(\vec{R})\Phi = - k^2\Phi \tag{1.2}$$

(k real) which at infinity ($\|\vec{R}\| \to \infty$) have the asymptotic behavior given by

$$\Phi_k(\vec{R}) \sim e^{ik\sqrt{2}z} + f_k(\vec{e})\, \frac{e^{ik\sqrt{2}\|\vec{R}\|}}{\|\vec{R}\|}, \tag{1.3}$$

where $\vec{e}$ is the unit vector in the $\vec{R}$ direction (i.e. $\vec{e} = \vec{R}/\|\vec{R}\|$) and $\|\vec{R}\|$ denotes the length of the vector $\vec{R}$. The exponential $\exp(ik\sqrt{2}z)$ represents an incident plane wave in the direction of the (arbitrarily chosen) z-axis and the second term on the right-hand side of (1.3) is the principal asymptotic part of the scattered wave. The coefficient $f_k(\vec{e})$ is called the

(1) Supported in part by AFOSR Grant 72-2187.
(2) Supported in part by NSF-MPS 75-09939.

scattering amplitude and

$$\sigma^2 = \int_{S(1)} |f_k(\vec{e})|^2 \, d\sigma \tag{1.4}$$

(where S(1) is the unit sphere) the *scattering cross-section.*

It is easy to show that $\Phi_k(\vec{R})$ satisfying (1.3) is the (unique) solution of the integral equation

$$\Phi_k(R) = e^{ik\sqrt{2}z} - \frac{1}{2\pi}\int \frac{e^{ik\sqrt{2}\|\vec{R}-\vec{r}\|}}{\|\vec{R}-\vec{r}\|} q(\vec{r})\Phi_k(\vec{r}) \, d\vec{r}, \tag{1.5}$$

and it follows that

$$f_k(\vec{e}) = -\frac{1}{2\pi}\int e^{ik\sqrt{2}\vec{r}.\vec{e}} q(\vec{r})\Phi_k(\vec{r}) \, d\vec{r}. \tag{1.6}$$

2. In the limit $k \to 0$ (low energy limit) the problem is greatly simplified since the integral equation (1.5) assumes the form

$$\Phi_0(\vec{R}) = 1 - \frac{1}{2\pi}\int \frac{\Phi_0(\vec{r})q(\vec{r})}{\|\vec{R}-\vec{r}\|} \, d\vec{r} \tag{2.1}$$

and the scattering amplitude becomes independent of $\vec{e}$

$$f_0(\vec{e}) = -\Gamma = -\frac{1}{2\pi}\int q(\vec{r})\Phi_0(\vec{r}) \, d\vec{r}. \tag{2.2}$$

The quantity Γ is called the *scattering length.*

The integral equation (2.1) is reminiscent of an integral equation which occurs in probabilistic potential theory (see e.g. [1]), and one can therefore expect that a probabilistic interpretation of the scattering length can be obtained.

Consider for $s > 0$ the quantity

$$G_s(\vec{R}) = s\int_0^\infty e^{-st} E\left\{ e^{-\int_0^t q(\vec{R}+\vec{r}(\tau))d\tau} \right\} dt \tag{2.3}$$

where $E\{\ \}$ is the Wiener expectation and $\vec{r}(\tau)$ ($\vec{r}(0) = 0$) the three-dimensional Wiener process.

It can then be shown (by imitating e.g. a similar derivation in [1]) that

$$G_s(\vec{R}) = 1 - \frac{1}{2\pi}\int \frac{e^{-\sqrt{2s}\|\vec{R}-\vec{r}\|}}{\|\vec{R}-\vec{r}\|} q(\vec{r})G_s(\vec{r}) \, d\vec{r} \tag{2.4}$$

and hence that

$$(2.5) \qquad \int (1 - G_s(\vec{R}))\, d\vec{R} = \frac{1}{s} \int q(\vec{r}) G_s(\vec{r})\, d\vec{r}.$$

Using (2.3) we rewrite (2.5) in the equivalent form

$$(2.6) \qquad \int_0^\infty e^{-st} \int E \left\{ 1 - e^{-\int_0^t q(\vec{R}+\vec{r}(\tau))d\tau} \right\} d\vec{R}\, dt = \frac{1}{s^2} \int q(r) G_s(r)\, dr.$$

From (2.4) and (2.1) we see that

$$(2.7) \qquad \lim_{s\to 0} G_s(\vec{r}) = \Phi_0(\vec{r})$$

and that therefore as $s \to 0$

$$(2.8) \qquad \int_0^\infty e^{-st} \int E \left\{ 1 - e^{-\int_0^t q(\vec{R}+\vec{r}(\tau))\, d\tau} \right\} d\vec{R}\, dt \sim \frac{2\pi\Gamma}{s^2}.$$

Applying a standard Tauberian theorem, we obtain

$$(2.9) \qquad \int E \left\{ 1 - e^{-\int_0^t q(\vec{R}+\vec{r}(\tau))\, d\tau} \right\} d\vec{R} \sim 2\pi\Gamma t,\ t \to \infty$$

or

$$(2.10) \qquad \Gamma = \frac{1}{2\pi} \lim_{t\to\infty} \frac{1}{t} \int E \left\{ 1 - e^{-\int_0^t q(\vec{R}+\vec{r}(\tau))\, d\tau} \right\} d\vec{r}$$

which gives a probabilistic interpretation of the scattering length.

3. The scattering length is closely related to the concept of capacity, a subject of extensive and profound researches of Professor Brelot, to whom this note is dedicated.

To see this, we go back to the integral equation (2.1) and rewrite it in the form

$$(3.1) \qquad \Phi_0(\vec{R})\sqrt{q(\vec{R})} = \sqrt{q(\vec{R})} - \frac{1}{2\pi} \int \frac{\sqrt{q(\vec{R})}\sqrt{q(\vec{r})}}{\|\vec{R} - \vec{r}\|}\, \Phi_0(\vec{R})\sqrt{q(\vec{r})}\, d\vec{r}.$$

Denoting by $\psi_n(\vec{r})$ the normalized eigenfunctions and by

λ_n the corresponding eigenvalues of the hermitian kernel

$$K(\vec{r}, \vec{R}) = \frac{1}{2\pi} \frac{\sqrt{q(\vec{R})}\sqrt{q(\vec{r})}}{\|\vec{R} - \vec{r}\|} \tag{3.2}$$

we obtain by simple formal calculations

$$\begin{aligned} \Gamma &= \frac{1}{2\pi} \int \Phi_0(\vec{R}) q(\vec{R})\, d\vec{R} \\ &= \frac{1}{2\pi} \sum_{n=1}^{\infty} \frac{\left(\int \psi_n(\vec{R})\sqrt{q(\mathrm{R})}\, d\vec{R}\right)^2}{1 + \lambda_n}. \end{aligned} \tag{3.3}$$

Let now Ω be a compact set which is the closure of its interior Ω_0 and let $q(\vec{R})$ be the indicator function of Ω and let, for $u > 0$, Γ_u be the scattering length of the potential $uq(\vec{R})$.

It follows from (3.3) that

$$\Gamma_u = \frac{1}{2\pi} \sum_{n=1}^{\infty} \frac{\left(\int_\Omega \psi_n(\vec{R})\, d\vec{R}\right)^2}{\frac{1}{u} + \lambda_n} \tag{3.4}$$

where the ψ_n and λ_n are the (normalized) eigenfunctions and eigenvalues of the kernel

$$\frac{1}{2\pi} \frac{1}{\|\vec{r} - \vec{\rho}\|}, \quad \vec{r}, \vec{\rho} \in \Omega.$$

It thas been shown in [1] that

$$\lim_{u \to \infty} \Gamma_n = \gamma, \tag{3.5}$$

where γ is equal to the classical capacity for a class of sets called semi-classical.

4. If we are dealing with a truly « hard potential » on Ω

$$q(\vec{R}) = \begin{cases} +\infty, & \vec{R} \in \Omega \\ 0, & \vec{R} \notin \Omega \end{cases} \tag{4.1}$$

we must interpret $\Phi_0(\vec{R})$ as 1 minus the usual capacitory potential of Ω. It is now easy to see that

$$(4.2)\quad E\left\{e^{-\int_0^t q(\vec{R}+\vec{r}(\tau))\,d\tau}\right\} = \text{Prob}\,\{\vec{R} + \vec{r}(\tau) \notin \Omega,\ 0 \leqslant \tau \leqslant t\},$$

and it was proved by Spitzer [2] that

$$(4.3)\quad \int d\vec{R}[1 - \text{Prob}\,\{\vec{R} + \vec{r}(\tau) \notin \Omega, 0 \leqslant \tau \leqslant t\}] \sim 2\pi C t, \quad t \to \infty$$

where C is the ordinary capacity of Ω.

Thus both the « semi-classical » capacity γ and the ordinary capacity C are related to the scattering length.

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Manuscrit reçu le 6 mars 1975.

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