Eidgenössische Technische Hochschule Zürich
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Isoperimetric Inequalities in a Boundary Value Problem in an Unbounded Domain

R. Sperb

Research Report No. 93-07
October 1993

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Abstract

In this paper a semilinear elliptic boundary value problem in the exterior of a finite domain is considered. An important example in applications is the Poisson-Boltzmann problem. Isoperimetric inequalities for a functional of the solution are proven using optimal sub- or supersolutions.

Keywords: Isoperimetric Inequalities, Poisson-Boltzmann Problem

Subject Classification: 35J60

1. Introduction

Let Ω be a bounded domain in $\mathbb{R}^N$, $N \geq 3$ and Ω^* the exterior of Ω. We consider the boundary value problem

$$\left.\begin{array}{rcl l l} \Delta u &=& \gamma^2 f(u) & \text{in} & \Omega^* \\ u &=& 1 & \text{on} & \partial\Omega \\ u &\to& 0 \ \text{ as } |x| \to \infty & & \end{array}\right\} . \tag{1.1}$$

Here x is a generic point of $\mathbb{R}^N$, γ is a given positive parameter and the nonlinearity is assumed to satisfy

$$f(0) = 0, \quad f'(0) > 0, \quad f''(u) \geq 0 \ \text{ for } \ u \geq 0 . \tag{1.2}$$

The assumptions on $f(u)$ guarantee that the solution decays to zero when $|x| \to \infty$ at least as fast as the solution of the linearised problem. Two possible backgrounds for problem (1.1) are described in the following:

(a) *Poisson-Boltzmann problem:*
With this application in mind u represents the potential of a charge distribution. Important choices for $f(u)$ are then

$$f(u) = \sin h\, u \ \text{ or } \ f(u) = u \text{ (Debye-Hückel approximation)} .$$

The parameter γ then involves a number of physical constants (see e.g. Garrett & Poladian [2]).

(b) *Reaction-Diffusion:*
In this interpretation u is the concentration of a reactant. The reactant is fed into Ω and diffuses through $\partial\,\Omega$ into the reaction region Ω^* where a simultaneous diffusion-reaction process takes place. The concentration inside Ω is held constant by a continuous supply of reactant. An important case is again $f(u) = u$ (e.g. for a first order degradation process). Another frequent choice is (Michaelis-Menten kinetics)

$$f(u) = \frac{u}{a+u}, \quad \text{where } a \text{ is a positive constant} .$$

Especially with the second interpretation of problem (1.1) in mind one is mostly not interested in the values $u(x)$, but rather in some functional of the solution. If (1.1) describes a diffusion reaction process then one has the relation

$$\gamma^2 = \frac{k}{D} ,$$

where k is the reaction rate and D the diffusion coefficient. Very often then (see Aris [1] one is interested in a pure number characterizing the influence of diffusion in the chemical reaction. One such possible number may be defined as

$$\eta := \frac{\oint_{\partial\Omega} |\nabla u| \, d\sigma}{\gamma^2 |\Omega|} . \tag{1.3}$$

Here $d\sigma$ is the surface element of $\partial\Omega$ and $|\Omega|$ the volume of Ω. We will concentrate mainly on optimal estimates for η in terms of geometrical data of Ω.

Note that for $\gamma = 0$ and the condition $u(x) = O(|x|^{2-N})$, for $|x| \to \infty$, $N \geq 3$, (1.1) is the classical electrostatic problem and $\oint_{\partial\Omega} |\nabla u| ds$ is up to normalization the electrostatic capacity of Ω.

2. Bounds derived from optimal sub- or supersolutions

Suppose we can find a function $\underline{u}(x)$ with the properties (subsolution)

$$\left.\begin{array}{rcl} \Delta \underline{u} & \geq & \gamma^2 f(\underline{u}) \ \text{ in } \Omega^* \\ \underline{u} & \leq & 1 \ \text{ on } \partial\Omega, \ \underline{u}(x) \to 0 \ \text{ for } \ |x| \to \infty \end{array}\right\} . \tag{2.1}$$

For the limiting case $\gamma = 0$ we have to replace the boundary condition at infinity by

$$\underline{u}(x) = O(|x|^{2-N}), \quad N \geq 3 \ (N = \ \text{Number of dimensions} \ .$$

Then one has $\underline{u}(x) \leq u(x)$ for any $x \in \Omega^*$. For a supersolution $\overline{u}(x)$ one just has to reverse all inequality signs.

In the following we construct an optimal subsolution in two steps. First we define $\varphi(\rho)$ as the solution of problem (1.1) for the exterior of an N-ball of radius R. It is easy to see that we can take $\varphi(\rho)$ as the solution of (prime denotes $\frac{d}{d\rho}$)

$$\left.\begin{array}{rcl} \frac{1}{\rho^{N-1}} \left(\rho^{N-1}\varphi'\right)' & = & (\gamma R)^2 f(\varphi) \ \text{ for } \ \rho \in (1, \infty) \\ \varphi(1) & = & 1, \ \varphi(\rho) \to 0 \ \text{ for } \rho \to \infty \end{array}\right\} . \tag{2.2}$$

The second important ingredient is the (exterior) distance function $d(x) = \min_{y \in \partial\Omega} |x - y|$, $x \in \Omega^*$. We then set

$$s(x) = \Big(1 + H_0 \, d(x)\Big)^{2-N}, \ N \geq 3 \ . \tag{2.3}$$

Here

$$H_0 = \max_{y \in \partial\Omega} \left\{ \frac{1}{N-1} \sum_{j=1}^{N-1} k_j(y) \right\} ,$$

where $k_j(y)$ denote the principal curvatures at a point y of $\partial\Omega$. Thus H_0 is the maximum of the mean curvature, which is assumed to be finite. Note that for the N-ball $H_0 = \frac{1}{R}$. The next result will enable us to derive optimal bounds for η as defined in Eq. (1.3).

Lemma 1 *Let Ω be a convex domain, i.e. $k_j \geq 0$ for $j = 1, ..., N-1$. Then the function $\underline{u}(x) = \widetilde{\varphi}(s(x))$, $s(x)$ defined by Eq. (2.3) and where $\widetilde{\varphi}(s) = \varphi(\rho)$, $\varphi(\rho)$ being the solution of (2.2) and $s = \frac{1}{\rho^{N-2}}$, is a subsolution to problem (1.1).*

In order to prove Lemma 1 it is convenient to prove first an auxiliary result stated as:

Lemma 2 *Let Ω be a convex domain. Then the function $s(x)$ defined in Eq. (2.3) satisfies $\Delta s \geq 0$ in Ω^*.*

Proof: We have

$$\Delta s = \frac{(2-N)\,H_0}{(1+H_0\,d)^{N-1}}\;\Delta d + \frac{(N-2)(N-1)}{(1+H_0\,d)^N}\;H_0^2 \cdot |\nabla d|^2 \;.$$

But one has (see e.g. Gibarg-Trudinger [3], p. 355)

$$\Delta d = \sum_{i=1}^{N-1}\;\frac{k_i}{1+k_i\,d}\;,\; |\nabla d| = 1\;,$$

so that

$$\Delta s = \frac{(N-2)\,H_0}{(1+H_0\,d)^N}\;\{(N-1)\,H_0 - (1+H_0\,d)\,\Delta d\}\;.$$

We now rewrite the term$\{(N-1)\,H_0 - (1-H_0\,d)\,\Delta d\}$ putting the expression for Δd over a common denominator. Then we may write

$$\Delta d = \frac{A(d)}{B(d)}\;,$$

with

$$A(d) = \sum_{j=0}^{N-1}\;j \cdot P_j\,d^{j-1},\;\; B(d) = \sum_{j=0}^{N-1}\;P_j \cdot d^j\;.$$

Here we have used the abbreviation P_j, where $P_0 \equiv 1$ and $P_j =$ sum of all products with j different factors k_ℓ and $1 \leq j,\, \ell \leq N-1$.

With this notation we can write

$$\Delta s = \frac{(N-2)\,H_0}{(1+H_0\,d)^N\,B(d)}\;\Big\{\underbrace{(N-1)\,H_0\,B(d) - (1+H_0\,d)\,A(d)}_{f(d)}\Big\}\;.$$

The expression $f(d)$ can be put into the form

$$f(d) = \sum_{\ell=0}^{N-1}\;C_\ell \cdot d^\ell\;,$$

where

$$C_\ell = H_0\,P_\ell\Big(1 - \frac{\ell}{N-1}\Big) - (\ell+1)\,P_{\ell+1}\;.$$

We finally show that $C_\ell \geq 0$ for all ℓ. It is clear for $\ell = 0$ and $\ell = N-1$, noting that by definition

$$P_1 = \sum_{j=1}^{N-1}\;k_j \leq (N-1)\,H_0\;.$$

We consider C_ℓ as a function of the $N-1$ variables k_j. Since C_ℓ is symmetric in all variables the minimum is attained for values k_j such that

$$k_1 = k_2 = ... = k_{N-1} = k^0 \ .$$

But

$$P_\ell(k^0, ..., k^0) = \binom{N-1}{\ell} (k^0)^\ell \ ,$$

and hence

$$C_\ell(k, ..., k_{N-1}) \geq C_\ell(k^0, ..., k^0) = 0 \ ,$$

which implies that $\Delta s \geq 0$.

Remarks on Lemma 2:

(a) For the special case $\gamma = 0$ Lemma 2 shows that

$$s(x) = (1 + H_0 \, d(x))^{2-N}$$

is a subsolution in the "capacity problem", i.e.

$$u(x) \geq (1 + H_0 \, d(x))^{2-N}, \quad N \geq 3 \ , \tag{2.4}$$

and the equality sign holds in (2.4) if Ω is the N-ball of radius $R = \frac{1}{H_0}$. Inequality (2.4) was derived by Payne & Philippin [4] by a different method.

(b) The convexity assumption is needed in order to ensure that Δd is finite for all $x \in \Omega^*$. Inequality (2.4) however holds without the convexity assumption, as shown by Payne & Philippin.

Proof of Lemma 1: We have

$$\Delta \overline{u} = \frac{d\widetilde{\varphi}}{ds} \cdot \Delta s + \frac{d^2\widetilde{\varphi}}{ds^2} \cdot |\nabla s|^2 \ ,$$

and

$$|\nabla s|^2 = \frac{((N-2) \, H_0)^2}{(1 + H_0 \, d)^{2N-2}} \, |\nabla s|^2 = \frac{((N-2) \, H_0)^2}{\rho^{2N-2}} \ . \tag{2.5}$$

Furthermore

$$\frac{d\widetilde{\varphi}}{ds} = \frac{1}{N-2} \, \rho^{N-1} \, \frac{d\varphi}{d\rho} \ , \tag{2.6}$$

and hence

$$\begin{aligned} \Delta \underline{u} - \gamma^2 f(\underline{u}) \ &\geq \ \frac{((N-2) \, H_0)^2}{\rho^{2N-2}} \ \frac{d^2\widetilde{\varphi}}{ds^2} - \gamma^2 f(\varphi) \\ &= \ \frac{H_0^2}{\rho^{N-1}} \ \frac{d}{d\rho} \ \left(\rho^{N-1} \, \frac{d\varphi}{d\rho}\right) - \gamma^2 f(\varphi) = 0 \ . \end{aligned}$$

On $\partial\Omega$ we have $\rho = 1$ and thus
$\underline{u} = \varphi(1) = 1$ on $\partial\Omega$
as well as
$u(x) \to 0$ as $|x| \to \infty$.

As a consequence of Lemma 1 we have

Theorem 1 *Let Ω be a finite convex domain in $\mathbb{R}^N$, $N \geq 3$. Denote by H_0 the maximum of the mean curvature of $\partial\Omega$ and by η_0 the effectiveness of a ball of radius H_0^{-1} (as defined by Eq. (1.3)). Then the effectiveness η of Ω satisfies*

$$\eta \leq \eta_0 \, \frac{|\partial\Omega|}{N H_0 |\Omega|} \tag{2.7}$$

and the equality sign holds if Ω is a ball.

Proof: Since the subsolution $\underline{u}$ defined in Lemma 1 satisfies the boundary conditions required in problem (1.1) we have

$$\oint_{\partial\Omega} |\nabla u| d\sigma \leq \oint_{\partial\Omega} |\nabla \underline{u}| d\sigma \; . \tag{2.8}$$

But from Eq. (2.5) and (2.6) we find

$$\oint_{\partial\Omega} |\nabla \underline{u}| d\sigma = -H_0 \cdot \frac{d\varphi}{d\rho}\Big|_{\rho=1} \cdot |\partial\Omega| \; . \tag{2.9}$$

From (2.2) it follows that ($R = H_0^{-1}$)

$$\eta_0 = \frac{N H_0^2}{\gamma^2} \, |\varphi'(1)| \; . \tag{2.10}$$

Eqs. (2.9) and (2.10) then imply inequality (2.7).

Remarks on Theorem 1

(a) An important case for applications is $N = 3$ and $f(u) = u$. Then the subsolution can be written down explicitly and one has at distance d from $\partial\Omega$

$$u(d) \geq \frac{e^{-\gamma d}}{1 + H_0 \, d} \; . \tag{2.11}$$

Inequality (2.7) then takes the form

$$\eta \leq \frac{(H_0 + \gamma)|\partial\Omega|}{\gamma^2 |\Omega|} \; . \tag{2.12}$$

(b) We can also derive an explicit lower bound for η from Lemma 1 in the case $N = 3, f(u) = u$. From the differential equation and the boundary conditions it follows that

$$\eta = \frac{1}{|\Omega|} \int_{\Omega^*} u\, dx \geq \frac{1}{|\Omega|} \int_{\Omega^*} \underline{u}\, dx \; .$$

We integrate over Ω^* using parallel surfaces to $\partial\Omega$. One has for the surface area $S(\delta)$ of a parallel surface at distance δ from $\partial\Omega$ (see e.g. Polya-Szegö [5], p.66)

$$S(\delta) = S(0) + 2M \cdot \delta + 4\pi\, \delta^2 \; . \tag{2.13}$$

Here M is the Minkowski constant of $\partial\Omega$ defined by

$$M = \int_{\partial\Omega} H\, d\sigma, \quad H = \text{mean curvature} \; , \tag{2.14}$$

and of course $S(0) = |\partial\Omega|$.

Hence we have

$$\eta \geq \frac{1}{|\Omega|} \int_0^\infty \frac{e^{-\gamma\delta}}{1 + H_0\, \delta} (|\partial\Omega| + 2M\delta + 4\pi\, \delta^2)\, d\sigma \; . \tag{2.15}$$

The evaluation of the integral gives after some routine calculation

$$\eta \geq \frac{1}{\nu} \left\{ \frac{4\pi}{\mu} + \lambda + \mu (H_0^2\, |\partial\Omega| - \lambda)\, e^\mu \cdot E_1(\mu) \right\} , \tag{2.16}$$

where the following abbreviations have been used:

$$\nu = H_0^2\, \gamma |\Omega|, \quad \mu = \frac{\gamma}{H_0}, \quad \lambda = 2M\, H_0 - 4\pi \; . \tag{2.17}$$

$E_1(\mu)$ denotes the exponential integral defined by

$$E_1(\mu) = \int_\mu^\infty \frac{e^{-t}}{t}\, dt \; .$$

Inequality (2.16) is again isoperimetric since the equality sign holds if Ω is a ball.

(c) One could also derive a version of Theorem 1 valid for plane domains Ω. However then the limiting case $\gamma = 0$ does not make any sense. In addition problem (1.1) seems less interesting in the two dimensional case.

Next we derive an estimate for η which is based on the construction of an optimal supersolution $\overline{u}$. For this purpose we use as an auxiliary problem the "electrostatic problem" ($N \geq 3$)

$$\left.\begin{array}{rcll} \Delta h & = & 0 & \text{in} \quad \Omega^* \\ h & = & 1 & \text{on} \quad \partial\Omega \\ h(x) & = & O(|x|^{2-N}) & \text{as} \quad |x| \to \infty \end{array}\right\} \tag{2.18}$$

In order to get an explicit inequality we restrict our attention to the special case $f(u) = u$.

Theorem 2 *Let $f(u) = u$ in problem (1.1) and Ω be a finite domain with boundary of class $C^{2+\epsilon}$, but not necessarily convex. Let $\tau = \max_{\partial\Omega} |\nabla h|$, h being the solution of (2.18), and $C = w_N^{-1} \oint_{\partial\Omega} |\nabla h| d\sigma$ the "capacity" of $\partial\Omega (w_N = (N-1)$ dimensional surface area of the unit N-sphere). Then we have*

$$\eta \geq \left[1 + \frac{\kappa}{N-2} \; \frac{K_{\frac{N-4}{2}}(\kappa)}{K_{\frac{N-2}{2}}(\kappa)}\right] \; \frac{C \cdot w_N}{\gamma^2 |\Omega|} \tag{2.19}$$

where $\kappa = (N-2) \frac{\gamma}{\tau}$ and $K_p(\kappa)$ denote Bessel functions. The equality sign holds if Ω is the N-ball.

Proof: We use the solution of (1.1) with $f(u) = u$ and Ω the unit ball as an auxiliary function:

$$\left.\begin{array}{rcll} \frac{1}{\rho^{N-1}} \left(\rho^{N-1} \varphi'(\rho)\right)' & = & c^2 \varphi & \text{in} \quad (1, \infty) \\ \varphi(1) & = & 1, \; \varphi(\rho) \to 0 & \text{for} \quad \rho \to \infty \end{array}\right\} . \tag{2.20}$$

The value of c will be chosen later. The solution of (2.20) is

$$\varphi(\rho) = \rho^{\frac{N-2}{2}} \cdot \frac{K_{\frac{N-2}{2}}(c\rho)}{K_{\frac{N-2}{2}}(c)} . \tag{2.21}$$

We then set $\rho = h^{-\frac{1}{N-2}}$, h being the solution of problem (2.18). It is convenient to write

$$\begin{array}{rcl} \hat{\varphi}(h) & = & \varphi(\rho) \;\; \text{and to use the relation} \\ \frac{d}{dh} & = & -\frac{1}{N-2} \, h^{-\frac{N-1}{N-2}} \; \frac{d}{d\rho} = -\frac{1}{N-2} \, \rho^{N-1} \; \frac{d}{d\rho} . \end{array} \tag{2.22}$$

We now choose $\overline{u}(x) = \varphi(\rho(x)) = \hat{\varphi}(h(x))$ and calculate

$$\Delta \overline{u} = \frac{d\hat{\varphi}}{dh} \cdot \Delta h + \frac{d^2 \hat{\varphi}}{dh^2} \cdot |\nabla h|^2 = \frac{d^2 \varphi}{dh^2} \cdot |\nabla h|^2 . \tag{2.23}$$

At this point we use a result of Payne & Philippin [4] stating that in N dimensions the solution h of (2.18) satisfies (the smoothness of $\partial\Omega$ is used here!)

$$|\nabla h|^2 \leq \tau^2 \cdot h^{\frac{2(N-1)}{N-2}} . \tag{2.24}$$

Hence

$$\Delta \overline{u} - \gamma^2 \overline{u} \leq \tau^2 \; \frac{d^2 \hat{\varphi}}{dh^2} \cdot h^{\frac{N-2}{2(N-1)}} - \gamma^2 \, \hat{\varphi} ,$$

but because of Eq. (2.22) this can be put into the form

$$\Delta \overline{u} - \gamma^2 \overline{u} \leq \frac{\tau^2}{(N-2)^2} \; \frac{1}{\rho^{2(N-1)}} \, \rho^{N-1} \; \frac{d}{d\rho} \left(\rho^{N-1} \; \frac{d\varphi}{d\rho}\right) - \gamma^2 \, \varphi(\rho) = 0 ,$$

if we choose $c = \frac{(N-2)\gamma}{\tau}$ in problem (2.20). It is easy to see that $\overline{u}$ satisfies the boundary conditions. We therefore have

$$\oint_{\partial\Omega} |\nabla u| d\sigma \geq \oint_{\partial\Omega} |\nabla \overline{u}| d\sigma \, . \tag{2.25}$$

The relations

$$\overline{u} = \sqrt{h}\, \frac{K_{\frac{N-2}{2}}(\kappa\, h^p)}{K_{\frac{N-2}{2}}(\kappa)}, \quad \kappa = \frac{(N-2)\gamma}{\tau}, \quad p = -\frac{1}{N-2}$$

together with well known identities for Bessel functions then show after some routine calculations that inequality (2.25) leads to the statement of Theorem 2.

Remarks on Theorem 2

(a) Inequality (2.19) is still not quite explicit. It is not hard to check that the function

$$s\, \frac{K_{\frac{N-4}{2}}(s)}{K_{\frac{N-2}{2}}(s)}$$

is increasing for $s > 0$. Hence we need an upper bound for τ and a lower bound for the capacity C. It was shown by Payne & Philippin [4] that

$$\tau \leq (N-2)\, H_0 \, . \tag{2.26}$$

For the capacity C one has the classical result of Poincaré-Szegö (see [6]) that

$$C \geq (N-2) \Big(\frac{N|\Omega|}{w_N} \Big)^{\frac{N-2}{N}} \, . \tag{2.27}$$

Inequality (2.19) therefore implies the weaker but still isoperimetric inequality

$$\eta \geq \left(1 + \frac{\gamma}{H_0} \cdot \frac{K_{\frac{N-4}{2}}\,(\frac{\gamma}{H_0})}{K_{\frac{N-2}{2}}\,(\frac{\gamma}{H_0})} \right) \frac{(N-2)}{\gamma^2 (\frac{N|\Omega|}{w_N})^{2/N}} \tag{2.28}$$

which for $N = 3$ reduces to

$$\eta \geq 3 \Big(\frac{1}{\gamma^2} + \frac{1}{\gamma\, H_0} \Big) \Big(\frac{4\pi}{3|\Omega|} \Big)^{2/3} \, . \tag{2.29}$$

(b) For $N = 3$ the supersolution $\overline{u}$ can be written as

$$\overline{u}(x) = h(x)\ \exp\Big\{ -\frac{\gamma}{\tau} \Big(\frac{1}{h(x)} - 1 \Big) \Big\} \, . \tag{2.30}$$

An explicit upper solution $\overline{h}(x)$ for $h(x)$ would then lead to an explicit upper bound for $\overline{u}(x)$. However for general domains it seems difficult to give an optimal choice of $\overline{h}(x)$.

3. Concluding Remarks

(a) The method of integration over level surfaces (see Sperb [7]) could also be used in order to derive an optimal inequality for the "effectiveness" η. One can show then that for given N-volume of Ω η is a minimum for the N-ball. In order to keep this note at a reasonable length we mention this result without proof.

(b) A number of additional bounds could be proven by exploiting the fact that the function

$$P := |\nabla u|^2 - 2\gamma^2 F(u) + \beta u \ ,$$

where $F(u) = \int_0^u f(v)dv$ and β is chosen appropriately, is non positive in Ω^*. Here techniques described in Sperb [7] can be used.

(c) The case $N = 2$ has been excluded here since it is of less interest in applications. It is however not hard to extend Theorem 1 (but not Theorem 2) to this case. Also for the remarks (a),(b) above the two-dimensional case is no exception.

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