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On the Schrödinger Equation and the Eigenvalue Problem

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Abstract. If λ_k is the k^{th} eigenvalue for the Dirichlet boundary problem on a bounded domain in $\mathbb{R}^n$, H. Weyl's asymptotic formula asserts that $\lambda_k \sim C_n\left(\frac{k}{V(D)}\right)^{2/n}$, hence $\sum_{i=1}^{k} \lambda_i \sim \frac{nC_n}{n+2} k^{\frac{n+2}{n}} V(D)^{-2/n}$. We prove that for any domain and for all k, $\sum_{i=1}^{k} \lambda_i \geqq \frac{nC_n}{n+2} k^{\frac{n+2}{n}} V(D)^{-2/n}$. A simple proof for the upper bound of the number of eigenvalues less than or equal to $-\alpha$ for the operator $\Delta - V(x)$ defined on $\mathbb{R}^n$ $(n \geqq 3)$ in terms of $\int_{\mathbb{R}^n} (V+\alpha)_-^{n/2}\, dx$ is also provided.

0. Introduction

In this paper, we study the eigenvalue problem with or without potential. We mainly concern ourself with bounded domains in $\mathbb{R}^n$ for the case of the Laplace operator. If D is a bounded domain in $\mathbb{R}^n$ we consider the eigenvalue problem

$$\Delta\phi = -\lambda\phi, \quad \text{on} \quad D$$

and

$$\phi|_{\partial D} \equiv 0. \tag{$*$}$$

The discreteness of the spectrum of Δ allows one to order the eigenvalues $(0<)\lambda_1 < \lambda_2 \leqq \ldots \leqq \lambda_k \leqq \ldots$, monotonically.

In the case of the Schrödinger equation, we consider potentials whose negative part are in $L^{n/2}(\mathbb{R}^n)$. If $V(x)$ is a potential function defined on $\mathbb{R}^n$ for $n \geqq 3$ and suppose $\int_{\mathbb{R}^n} V_-(x)\, dx$ is finite (see Sect. 2 for definition), it is then well known that the operator $\Delta - V(x)$ has discrete spectrum on the negative real line, i.e., the number of non-positive eigenvalues $N(0)$ for the problem

$$(\Delta - V(x))\,\phi(x) = -\mu\phi(x), \quad \text{on} \quad \mathbb{R}^n \tag{$**$}$$

is finite.

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Before we state our results, we would like to remark on the history of both problems (*) and (**). In 1912, H. Weyl proved that the spectrum of (*) has the following asymptotic behavior as $k \to \infty$,

$$\lambda_k \sim C_n \left(\frac{k}{V}\right)^{2/n},$$

where $V =$ volume of D, and $C_n = (2\pi)^2 B_n^{-2/n}$, with $B_n =$ volume of the unit n-ball. One calls the constant C_n to be the Weyl constant or the "classical constant." Pólya in his paper [6] dedicated to Weyl (in 1960) proved that for any "plane-covering domain" D in $\mathbb{R}^2$ (those that tile $\mathbb{R}^2$)

$$\lambda_k \geqq C_n \left(\frac{k}{V}\right)^{2/n}, \quad \text{for all} \quad k.$$

He then conjectured that the inequality should hold for general domain D in $\mathbb{R}^2$. We should like to point out that his proof applied to $\mathbb{R}^n$-covering domains also.

In 1980, Lieb [4] proved that there exist constants $\tilde{C}_n$, such that

$$\lambda_k \geqq \tilde{C}_n \left(\frac{k}{V}\right)^{2/n}$$

for any domain $D \subseteqq \mathbb{R}^n$. However C_n differs from $\tilde{C}_n$ by a factor.

The first part of this paper is devoted to proving that

$$\lambda_k \geqq \frac{nC_n}{n+2} \left(\frac{k}{V}\right)^{2/n}$$

for all $k \geqq 1$ and for any domain $D \subseteqq \mathbb{R}^n$. In fact, we will show that

$$\sum_{i=1}^{k} \lambda_i \geqq \frac{nC_n}{n+2} k^{\frac{n+2}{n}} V^{\frac{-2}{n}}$$

for all $k \geqq 1$ and for any $D \subseteqq \mathbb{R}^n$. Although we are unsuccessful in proving Pólya's conjecture, the lower bound of $\sum_{i=1}^{k} \lambda_i$ however is sharp since

$$\sum_{i=1}^{k} \lambda_i \sim \frac{nC_n}{n+2} k^{\frac{n+2}{n}} V^{\frac{-2}{n}}$$

in view of H. Weyl's asymptotic formula.

In our original proof, the constant we obtained was $\frac{2\pi n}{e}$ instead of $\frac{nC_n}{n+2}$, which also has the property that

$$\lim_{n \to \infty} \frac{2\pi n}{eC_n} = 1.$$

After reading the first version of our manuscript, Lars Hörmander informed us of Lemma 1. This enabled us to shorten our proof to the present form and also improved our constant to $\frac{nC_n}{n+2}$. The authors would like to take this opportunity to acknowledge our gratitude to Hörmander.

As for the second problem (**), the quantity $N(\alpha) = \#$ {eigenvalues $\leqq -\alpha$, for $\alpha \geqq 0$} is referred to, by physicists, as the number of bound states when $\alpha = 0$. In 1972, Rosenbljum announced his estimates of $N(\alpha)$ by the $L^{n/2}$-norm of $(V+\alpha)_-$ (when $n \geqq 3$) in a Russian journal [7]. Meanwhile in America, unaware of Rosenbljum's result, Simon [8] derived a slightly weaker estimate and posed the question regarding the validity of the inequality

$$\bar{C}_n N(\alpha) \leqq \int_{\mathbb{R}^n} (V+\alpha)_-^{n/2} \, dx$$

for $n \geqq 3$. In the same year, Cwikel and Lieb [3, 4, 9] independently proved the above inequality. The sharpest constant $\bar{C}_n$ so far was due to Lieb. He then conjectured that the best constant for such an inequality when $n=3$ should be

$$\left(\frac{n(n-2)}{4}\right)^{n/2} \omega_{n-1} .$$

The second part of this paper is to establish the estimate

$$\left(\frac{n(n-2)}{4e}\right)^{n/2} \omega_{n-1} N(\alpha) \leqq \int_{\mathbb{R}^n} (V+\alpha)_-^{n/2} \, dx .$$

This constant seems to be the sharpest among all existing estimates and we also believe our method is the simplest. Moreover, it might be worth pointing out that our estimate is valid on a manifold where the constant will depend on the Sobolev constant. Finally, we remark that when $n=2$, the inequality is false, and counterexamples are known.

1. Lower Bounds for λ_k

In this section, we study the first problem (*) stated in Sect. 0. The technique being employed is motivated by a paper of Cheng and the first author [2]. We will begin by proving the following lemma which was pointed out to us by L. Hörmander.

Lemma 1. *If f is a real-valued function defined on $\mathbb{R}^n$ with $0 \leqq f \leqq M_1$, and*

$$\int_{\mathbb{R}^n} |z|^2 f(z) \, dz \leqq M_2 ,$$

then

$$\int_{\mathbb{R}^n} f(z) \, dz \leqq (M_1 B_n)^{\frac{2}{n+2}} M_2^{\frac{n}{n+2}} \left(\frac{n+2}{n}\right)^{\frac{n}{n+2}} ,$$

where B_n = volume of the unit n-ball in $\mathbb{R}^n$.

Proof. Let $g(z)=M_1$ when $|z|<R$ and $g(z)=0$ when $|z|\geqq R$ where R is chosen so that

$$\int |z|^2 g(z)\,dz = M_2.$$

Then $(|z|^2-R^2)(f(z)-g(z))\geqq 0$, hence

$$R^2\int (f(z)-g(z))\,dz < \int |z|^2(f(z)-g(z))\,dz = 0.$$

Now we have

$$M_2=\int_{\mathbb{R}^n} |z|^2 g(z)\,dz = M_1\int_0^R r^{n+1}\omega_{n-1}\,dr = M_1(\omega_{n-1}/(n+2))R^{n+2}$$

where $\omega_{n-1}=$ volume of the unit $(n-1)$ sphere in $\mathbb{R}^n$, and $\int g(z)\,dz = M_1 B_n R^n$. Hence using $nB_n=\omega_{n-1}$ we conclude that

$$\int f(z)\,dz \leqq \int g(z)\,dz = (M_1 B_n)^{\frac{2}{n+2}} M_2^{\frac{n}{n+2}} \left(\frac{n+2}{n}\right)^{\frac{n}{n+2}},$$

after solving for R.

Theorem 1. *Let D be a bounded domain in $\mathbb{R}^n$. Suppose λ_k denotes the k^{th} eigenvalue of D for the Dirichlet boundary problem. If V is the volume of D, then*

$$\sum_{i=1}^{k}\lambda_i \geqq \frac{nC_n}{n+2} k^{\frac{2+n}{n}} V^{\frac{-2}{n}}.$$

Proof. Let $\{\phi_i\}_{i=1}^k$ be the set of orthonormal eigenfunctions for the eigenvalues $\{\lambda_i\}_{i=1}^k$. We consider the function defined by

$$\Phi(x,y)=\sum_{i=1}^{k}\phi_i(x)\,\phi_i(y) \tag{1}$$

for $x, y\in D$. The Fourier transform of Φ in the x-variable is then given by

$$\hat{\Phi}(z,y)=(2\pi)^{-n/2}\int_{x\in\mathbb{R}^n}\Phi(x,y)e^{ix\cdot z}\,dx. \tag{2}$$

It has the standard property that

$$\int_{\mathbb{R}^n}\Phi^2(x,y)\,dx=\int_{\mathbb{R}^n}|\hat{\Phi}|^2(z,y)\,dz. \tag{3}$$

Hence

$$\int_{\mathbb{R}^n}\int_{\mathbb{R}^n}|\hat{\Phi}|^2(z,y)\,dz\,dy=\int_D\int_{\mathbb{R}^n}\Phi^2(x,y)\,dx\,dy$$

$$=\int_D\int_D\Phi^2(x,y)\,dx\,dy=k \tag{4}$$

by the orthonormality of $\{\lambda_i\}_{i=1}^k$.

On the other hand,

$$\int_{\mathbb{R}^n} |\hat{\Phi}|^2(z,y)\,dy = \int_D (2\pi)^{-n}\left|\int_{\mathbb{R}^n} \Phi(x,y)e^{ix\cdot z}\,dx\right|^2 dy$$
$$= \int_D (2\pi)^{-n}\left|\int_D \Phi(x,y)e^{ix\cdot z}\,dx\right|^2 dy\,. \tag{5}$$

By the definition of $\Phi(x,y)$, this is nothing more than a multiple by $(2\pi)^{-n}$ of the L^2-norm of the projection of the function $h(x)=e^{ix\cdot z}$ onto the subspace $\langle\lambda_i\rangle_{i=1}^k$ spanned by the first k^{th} eigenfunctions. Hence

$$\int_D |\hat{\Phi}|^2(z,y)\,dy \leqq (2\pi)^{-n}\int_D |e^{ix\cdot z}|^2\,dx = (2\pi)^{-n}V, \tag{6}$$

which is the L^2-norm of $h(x)$.

Meanwhile, we consider the equalities

$$z_j\hat{\Phi}(z,y) = (2\pi)^{-n/2}\int_{\mathbb{R}^n} \Phi(x,y)z_j e^{ix\cdot z}\,dx$$
$$= (2\pi)^{-n/2}\int_D \Phi(x,y)(-i)\frac{\partial}{\partial x_j}e^{ix\cdot z}\,dx$$
$$= i(2\pi)^{-n/2}\int_D\left(\frac{\partial}{\partial x_j}\Phi(x,y)\right)e^{ix\cdot z}\,dx$$
$$= i\widehat{\frac{\partial}{\partial x_j}\Phi}(z,y)\,, \tag{7}$$

which implies that

$$\int_{\mathbb{R}^n}\int_D |z|^2|\hat{\Phi}|^2(z,y)\,dy\,dz = \int_{\mathbb{R}^n}\int_D |\widehat{\nabla_x\Phi}|^2(z,y)\,dy\,dx$$
$$= \int_{\mathbb{R}^n}\int_D |\nabla_x\Phi|^2(x,y)\,dy\,dx$$
$$= -\int_D\int_D \Phi(x,y)\,\Delta_x\Phi(x,y)\,dy\,dx$$
$$= \sum_{i=1}^k \lambda_i \tag{8}$$

by definition of Φ.

Now, we can apply Lemma 1 to the function

$$f(z) = \int_D |\hat{\Phi}(z,y)|^2\,dy$$

with $M_1=(2\pi)^{-n}V$ and $M_2=\sum_{i=1}^k \lambda_i$ by (6) and (7). We conclude that

$$k = \int_{\mathbb{R}^n} f(z)\,dz \leqq ((2\pi)^{-n}VB_n)^{\frac{2}{n+2}}\left(\frac{n+2}{n}\right)^{\frac{n}{n+2}}\left(\sum_{i=1}^k \lambda_i\right)^{\frac{n}{n+2}}, \tag{9}$$

hence

$$\sum_{i=1}^{k} \lambda_i \geqq \frac{nC_n}{n+2} k^{\frac{n+2}{n}} V^{-2/n}.$$

Corollary 1. *Let D be a bounded domain in* $\mathbb{R}^n$. *Suppose* λ_k *denotes the* k^{th} *eigenvalues of D for the Dirichlet boundary problem. If V is the volume of D, then*

$$\lambda_k \geqq \frac{nC_n}{n+2} k^{2/n} V^{-2/n}.$$

Proof. Obvious.

2. Upper Bound for $N(\alpha)$

We will derive the upper bound for $N(\alpha)$ for the second problem stated in Sect. 0. We must point out that the reduction argument (Corollary 2) was first observed by Birman and Schwinger and was employed in [4]. The reduction, though simple, provides the key link to our argument which enables us to apply the next theorem about eigenvalues of the operator

$$\frac{\Delta_x}{q(x)}$$

with $q(x) > 0$.

Theorem 2. *Let D be a bounded domain in* $\mathbb{R}^n$ *for* $n \geqq 3$. *Suppose* $q(x)$ *is a positive function defined on D. Let* μ_k *be the* k^{th} *eigenvalue for the equation*

$$\Delta\psi(x) = -\mu q(x)\psi(x)$$

on D with Dirichlet boundary condition

$$\psi|_{\partial D} \equiv 0.$$

Then

$$\mu_k^{n/2} \int_D q^{n/2}(x)\,dx \geqq k\left(\frac{n(n-2)}{4e}\right)^{n/2} \omega_{n-1},$$

where ω_{n-1} = *volume of the unit* $(n-1)$-*sphere.*

Proof. We consider the "heat" kernel for the corresponding parabolic operator

$$\frac{\Delta}{q} - \frac{\partial}{\partial t}. \tag{10}$$

If $\{\psi_i(x)\}_{i=1}^{\infty}$ is a set of orthonormal eigenfunctions satisfying

$$\Delta\psi_i = -\mu_i q \psi_i$$

with eigenvalues $\{\mu_i\}$, then the kernel of (10) must take the form

$$H(x,y,t) = \sum_{i=1}^{\infty} e^{-\mu_i t}\psi_i(x)\psi_i(y). \tag{11}$$

It has the property that

$$H(x,y,t)>0$$

in the interior of $D\times D$, and

$$H(x,y,t)\equiv 0$$

on $\partial D\times\partial D$ for all t.

Note that our L^2-norm is given by the volume form $q(x)\,dx$ instead of dx, and the orthonormality of the ϕ_i's is with respect to this new volume form, i.e.,

$$\int_D \psi_i(x)\,\psi_j(x)\,q(x)\,dx=\delta_{ij}\,. \tag{12}$$

Let us consider the function

$$\begin{aligned} h(t) &= \sum_{i=1}^{\infty} e^{-2\mu_i t} \\ &= \int_D\int_D H^2(x,y,t)\,q(x)\,q(y)\,dx\,dy\,. \end{aligned} \tag{13}$$

Its t-derivative is given by

$$\begin{aligned} \frac{\partial h}{\partial t} &= 2\int_D\int_D H(x,y,t)\,q(x)\,q(y)\frac{\partial H}{\partial t}(x,y,t)\,dx\,dy \\ &= 2\int_D\int_D H(x,y,t)\,\Delta_y H(x,y,t)\,q(x)\,dy\,dx \\ &= -2\int_D q(x)\int_D |\nabla_y H(x,y,t)|^2\,dy\,dx\,. \end{aligned} \tag{14}$$

Here we have used the fact that $H(x,y,t)$ satisfy

$$\left(\frac{\Delta_y}{q(y)}-\frac{\partial}{\partial t}\right)H(x,y,t)\equiv 0\,.$$

On the other hand,

$$\begin{aligned} h(t) &= \int_D q(x)\int_D H^2(x,y,t)\,q(y)\,dy\,dx \\ &\leqq \int_D q(x)\left[\left(\int_D H^{\frac{2n}{n-2}}(x,y,t)\,dy\right)^{\frac{n-2}{n+2}}\left(\int_D H(x,y,t)\,q^{\frac{n+2}{4}}(y)\,dy\right)^{\frac{4}{n+2}}\right]dx \\ &\leqq \left[\int_D q(x)\left(\int_D H^{\frac{2n}{n-2}}(x,y,t)\,dy\right)^{\frac{n-2}{n}}dx\right]^{\frac{n}{n+2}} \\ &\quad\cdot\left[\int_D q(x)\left(\int_D H(x,y,t)\,q^{\frac{n+2}{4}}(y)\,dy\right)^2 dx\right]^{\frac{2}{n+2}}. \end{aligned} \tag{15}$$

The second term on the right hand side of (15) can be estimated as follows: We observe that the function

$$Q(x,t)=\int_D H(x,y,t)\,q^{\frac{n+2}{4}}(y)\,dy$$

satisfies the equation

$$\left(\frac{\Delta_x}{q(x)} - \frac{\partial}{\partial t}\right) Q(x,t) \equiv 0,$$

with $Q(x,t)\equiv 0$ on ∂D for $t>0$ and $Q(x,0)=q^{\frac{n-2}{4}}(x)$.

Computing

$$\begin{aligned}\frac{\partial}{\partial t}\int_D Q^2(x,t)\,q(x)\,dx &= 2\int_D Q(x,t)\frac{\partial Q}{\partial t}(x,t)\,q(x)\,dx\\ &= 2\int_D Q(x,t)\,\Delta_x Q(x,t)\,dx\\ &= -2\int_D |\nabla_x Q(x,t)|2\,dx\\ &\leqq 0. \end{aligned} \tag{16}$$

Hence

$$\begin{aligned}\int_D Q^2(x,t)\,q(x)\,dx &\leqq \int_D Q^2(x,0)\,q(x)\,dx\\ &= \int_D q^{n/2}(x)\,dx, \end{aligned} \tag{17}$$

and (15) takes the form

$$h^{\frac{n+2}{n}}(t)\left(\int_D q^{n/2}(x)\,dx\right)^{-2/n} \leqq \int_D q(x)\left(\int_D H^{\frac{2n}{n-2}}(x,y,t)\,dy\right)^{\frac{n-2}{n}} dx. \tag{18}$$

The Sobolev inequality asserts that for functions f with compact support in $\mathbb{R}^n$ (for $n\geqq 3$) must satisfy

$$\int_{\mathbb{R}^n} |\nabla f|^2 \geqq \frac{n(n-2)}{4}\,\omega_{n-1}^{2/n}\left(\int_{\mathbb{R}^n} |f|^{\frac{2n}{n-2}}\right)^{\frac{n-2}{n}}, \tag{19}$$

where ω_{n-1} is the volume of the unit $(n-1)$-sphere in $\mathbb{R}^n$. Hence together with (14) and (18) yield

$$\frac{\partial h}{\partial t} \leqq -\frac{n(n-2)}{2}\,\omega_{n-1}^{2/n}\left(\int_D q^{n/2}(x)\,dx\right)^{-2/n} h^{\frac{n+2}{n}}(t). \tag{20}$$

We must remark that the sharp constant in (19) was independently computed in [1] and [5].

Dividing (20) by $h^{\frac{n+2}{n}}(t)$ and integrating with respect to t, we have

$$h(t) \leqq (n-2)^{-n/2}\,\omega_{n-1}^{-1}\left(\int_D q^{n/2}(x)\,dx\right) t^{-n/2}.$$

By (13),

$$(n-2)^{-n/2}\,\omega_{n-1}^{-1}\left(\int_D q^{n/2}(x)\,dx\right) t^{-n/2} \geqq \sum_{i=1}^{\infty} e^{-2\mu_i t}.$$

Setting $t=\frac{n}{4\mu_k}$, we obtain

$$(n-2)^{-n/2}\omega_{n-1}^{-1}\left(\int_D q^{n/2}(x)\,dx\right)\left(\frac{n}{4}\right)^{-n/2}\mu_k^{n/2} \geqq \sum_{i=1}^{\infty} \exp\left(-\frac{n\mu_i}{2\mu_k}\right)$$
$$\geqq ke^{-n/2},$$

which is to be proved.

We will now utilize Theorem 2 to estimate the number of bound states for the Schrödinger equation. Let $V(x)$ be a function defined on $\mathbb{R}^n$ for $n \geqq 3$. We define

$$(V+\alpha)_-(x)=\begin{cases} -(V+\alpha)(x) & \text{if} \quad V(x)+\alpha \leqq 0 \\ 0 & \text{otherwise} \end{cases}$$

for $\alpha \geqq 0$. Let $N(\alpha)$ be the number of eigenvalues λ satisfying

$$(\Delta - V(x))\,\phi(x) = -\lambda\phi(x)$$

with $\lambda \leqq -\alpha$.

Corollary 2. $N(\alpha)\left(\frac{n(n-2)}{4e}\right)^{n/2} \omega_{n-1} \leqq \int_{\mathbb{R}^n} (V+\alpha)_-^{n/2}\,dx.$

Proof. The proof consists of a series of reduction procedures, most of which are standard. The goal is to reduce the problem to where Theorem 2 can be applied. Since these arguments are known, we will only outline their proofs.

(i) It suffices to show that

$$N(0)\left(\frac{n(n-2)}{4e}\right)^{n/2} \omega_{n-1} \leqq \int_{\mathbb{R}^n} V_-^{n/2}\,dx. \tag{21}$$

Indeed, to prove the inequality for arbitrary $\alpha \geqq 0$, we let $\tilde{V}(x)=V(x)+\alpha$. Applying (21) to the potential $\tilde{V}$ and observing that any number λ is an eigenvalue for $\Delta - V$ iff $\lambda+\alpha$ is an eigenvalue for $\Delta - \tilde{V}$, we establish the general form.

(ii) We may assume $V(x)<0$ for all $x \in \mathbb{R}^n$. By monotonicity of $N(0)$ with respect to the potential $V(x)$, we may assume $V(x) \leqq 0$ by replacing $V(x)$ by $-V_-(x)$. Approximating $-V_-(x)$ by a sequence of strictly negative functions in $L^{n/2}$-norm, obviously $V(x)<0$ can be assumed.

(iii) Exhausting $\mathbb{R}^n$ by compact subdomains, we only need to prove the inequality

$$N(0)\left(\frac{n(n-2)}{4e}\right)^{n/2} \omega_{n-1} \leqq \int_D V_-^{n/2}\,dx \tag{22}$$

for the Schrödinger equation on D given by

$$(\Delta - V)\phi = -\lambda\phi \quad \text{and} \quad \phi|_{\partial D} \equiv 0 \tag{23}$$

for any given domain $D \subseteqq \mathbb{R}^n$.

(iv) The number of non-positive eigenvalues $N(0)$ for (23) is equal to the number of eigenvalues less than 1 for the problem in Theorem 2 with $q(x) = -V(x)$.

To see this, we consider the quadratic form associated to (23),

$$\frac{\int|\nabla\phi|^2+\int V\phi^2}{\int\phi^2}=\frac{\int|V|\phi^2}{\int\phi^2}\left[\frac{\int|\nabla\phi|^2}{\int|V|\phi^2}-1\right]. \tag{24}$$

Hence the dimension of the dimension of the subspace on which the left hand side is non-positive is equal to the dimension of the subspace on which the quadratic form

$$\frac{\int|\nabla\phi|^2}{\int|V|\phi^2}$$

is less than or equal to 1. However the latter is the quadratic form associated to the operator in Theorem 2.

(v) To conclude the proof of the corollary, we set μ_k to be the greatest eigenvalue less than or equal to 1. Then Theorem 2 gives

$$\begin{aligned}\int_D |V|^{n/2}dx &\geqq \mu_k^{n/2}\int_D |V|^{n/2}dx\\ &\geqq k\left(\frac{n(n-2)}{4e}\right)^{n/2}\omega_{n-1}\\ &\geqq N(0)\left(\frac{n(n-2)}{4e}\right)^{n/2}\omega_{n-1}.\end{aligned}$$

This concludes the proof of Corollary 2.

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