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Lower Bounds and Isoperimetric Inequalities for Eigenvalues of the Schrödinger Equation*

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The potential which minimizes the lowest eigenvalue of the one-dimensional Schrödinger equation is determined among all potentials V for which the integral of V^n has the prescribed value k. For each value of n and k this potential is found to be a special case of the Epstein-Eckart potentials which were originally introduced because the Schrödinger equation for them could be solved explicitly. The minimum eigenvalue is determined and it provides a lower bound on the lowest eigenvalue of any potential for which $\int V^n dx = k$. The expression of this fact as an inequality yields an isoperimetric inequality. For an arbitrary potential, each value of n provides one lower bound on the lowest eigenvalue, the largest of which is the best. This best bound is determined for the square well, the exponential, and the inverse power potentials. In the case of the square well, it is compared with the exact value. In the limiting case $n=1$ our result reduces to that previously obtained by Larry Spruch, who showed that the delta function has the minimum lowest eigenvalue among all potentials of given "area."

1. INTRODUCTION

UPPER bounds on the lowest eigenvalue of the Schrödinger equation can be obtained easily because this eigenvalue is the minimum of a certain variational expression. However, it is not so easy to obtain lower bounds, although various methods have been devised for obtaining them. Therefore, we have re-examined the problem of obtaining lower bounds from a different viewpoint, i.e., that of isoperimetric inequalities. We seek that potential which in a specified class of potentials, yields the minimum lowest eigenvalue. Once we find it, its lowest eigenvalue is a lower bound on the lowest eigenvalue of all the potentials in the specified class. The resulting inequality is called an isoperimetric inequality by analogy with the classical inequality $A \leq L^2/4\pi$ relating the length of a curve to the area A it encloses. This classical isoperimetric inequality is a consequence of the fact that of all closed curves of length L, the circle encloses the greatest area $L^2/4\pi$.

Our analysis is confined to the one-dimensional case. We consider a two-parameter family of classes of potentials and, therefore, we obtain a one-parameter family of isoperimetric inequalities. Thus, we obtain a one parameter family of lower bounds on the lowest eigenvalue of a given potential. These bounds are explicit formulas, each merely involving an integral of some power of the potential. Naturally, the largest of the lower bounds is the best, but which is largest depends upon the potential. To illustrate the accuracy of the bounds, we determine the best one for a square well and compare it with the exact eigenvalue. We also obtain the best lower bound for exponential and inverse power potentials. In principle, our method applies to higher-dimensional cases, but it then leads to nonlinear differential equations which cannot be solved explicitly, whereas they can be solved explicitly in the one-dimensional case. These equations are given and some consequences of them are presented.

One interesting aspect of our results is that the potentials which yield the minimum lowest eigenvalues, in the classes we have considered, are special cases of the potentials introduced by Epstein. Their potentials were introduced because they led to Schrödinger equations which could be solved explicitly in terms of known functions.

The present investigation was undertaken to generalize the result, proved by Larry Spruch (unpublished), that the delta function has the smallest lowest eigenvalue of all potentials of given "area," i.e., of given integral of the magnitude of the potential. His result appears as a limiting case of our results. Our method of analysis is one which was devised previously to determine the shape of the strongest column of given length and volume.[2,3] In the course of the analysis, we also make use of a suggestion of H. F. Weinberger. In the final section we show by the same method that the usual upper bound for the lowest eigenvalue also results from an isoperimetric inequality.

2. ISOPERIMETRIC PROBLEM

The one-dimensional Schrödinger equation for the wave function $u(x)$ of a particle of energy λ in a potential $-V(x)$ is, in appropriate units,

$$u_{xx} + V(x)u + \lambda u = 0. \qquad (1)$$

This equation has a quadratically integrable solution if and only if λ has one of a discrete set of values called eigenvalues, which depend upon $V(x)$. We seek the potentials $V(x)$ which make stationary some eigenvalue

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[1] P. S. Epstein, Proc. Nat. Acad. Sci. **16**, 627 (1930).
[2] J. B. Keller, Archive Ratl. Mech. and Anal. **5**, 275 (1960).
[3] I. Tadjbaksh and J. B. Keller, *Strongest Columns and Isoperimetric Inequalities for Eigenvalues*, J. Appl. Mech. (to be published).

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λ of Eq. (1) among all potentials satisfying the condition

$$\int_{-\infty}^{\infty} V^n(x)dx = k. \qquad (2)$$

Here n and k are two real constants which characterize the class of potentials under consideration.

Let us suppose that $V_0(x)$ is a solution of this problem and that $u_0(x)$ and λ_0 are the corresponding eigenfunction and stationary eigenvalue. We introduce a family of potentials $V(x,\epsilon)$ depending smoothly upon a parameter ϵ, satisfying Eq. (2), and such that $V(x,0) = V_0(x)$. Then the corresponding eigenfunction $u(x,\epsilon)$ can be so normalized that it, as well as the eigenvalue $\lambda(\epsilon)$, depends smoothly upon ϵ. If we denote differentiation with respect to ϵ by a dot, it follows that $\dot{\lambda}(0)=0$. We now differentiate Eq. (1) and (2) with respect to ϵ and obtain

$$\dot{u}_{xx} + V\dot{u} + \lambda\dot{u} = -\dot{\lambda}u - \dot{V}u \qquad (3)$$

$$\int_{-\infty}^{\infty} V^{n-1}\dot{V}dx = 0. \qquad (4)$$

The inhomogeneous equation (3) has a quadratically integrable solution only if the right-hand side is orthogonal to u, the solution of Eq. (1). But since $u(x,\epsilon)$ is a smooth function of ϵ which is quadratically integrable, it follows that $\dot{u}$ exists and is also quadratically integrable. Therefore, the orthogonality condition is satisfied and it yields, when $\epsilon=0$,

$$\int_{-\infty}^{\infty} u_0^2\dot{V}dx = 0. \qquad (5)$$

The choice of $V(x,\epsilon)$ is arbitrary except that $V(x,0) = V_0(x)$, that it be a smooth function of ϵ and satisfy Eq. (2). Therefore, $\dot{V}$ is arbitrary except that it must satisfy Eq. (4). Thus Eq. (5) expresses the fact that u_0^2 is orthogonal to every function $\dot{V}$ which, by Eq. (4), is orthogonal to V_0^{n-1}. This implies that u_0^2 is a constant multiple of V_0^{n-1}. We shall choose the multiplier to be unity, since u can be multiplied by a constant factor and remain a solution of Eq. (1). Thus we have

$$u_0^2 = V_0^{n-1}. \qquad (6)$$

Let us now eliminate V_0 from Eq. (1) by means of Eq. (6), and obtain the following nonlinear equation for u_0:

$$u_{0xx} + u_0^{1+(2/n-1)} + \lambda_0 u_0 = 0. \qquad (7)$$

To solve Eq. (7) we multiply it by u_{0x} and integrate, obtaining

$$u_{0x}^2 + \frac{(n-1)}{n}u_0^{2+(2/n-1)} + \lambda_0 u_0^2 = 0. \qquad (8)$$

The integration constant has been set equal to zero in Eq. (8), since u_0 and u_{0x} must vanish when x becomes infinite, in order that u_0 be an eigenfunction. From Eq. (8) we find

$$u_{0x} = (-\lambda_0)^{\frac{1}{2}} u_0 \left(1 + \frac{n-1}{n\lambda} u_0^{2/n-1}\right)^{\frac{1}{2}}. \qquad (9)$$

To evaluate the integral which occurs in solving Eq. (9), it is convenient to replace u_0 by V_0 by means of Eq. (6). Then Eq. (9) becomes

$$V_{0x} = \frac{2(-\lambda)^{\frac{1}{2}}}{n-1} V_0 \left(1 + \frac{n-1}{n\lambda_0} V_0\right)^{\frac{1}{2}}. \qquad (10)$$

The various solutions of Eq. (10) differ only by translations. We shall select that solution for which $V_0(0) = n/(n-1)$. Then Eq. (10) yields

$$\frac{2(-\lambda_0)^{\frac{1}{2}}}{n-1}x = \int_{n/n-1}^{V_0} V^{-1}\left(1+\frac{n-1}{n\lambda_0}V\right)^{-\frac{1}{2}} dV$$

$$= -2\tanh^{-1}\left(1+\frac{n-1}{n\lambda_0}V_0\right)^{\frac{1}{2}}. \qquad (11)$$

Upon solving Eq. (11) for V_0, we obtain

$$V_0(x) = \frac{-n\lambda_0}{n-1}\,\text{sech}^2\left[\frac{(-\lambda_0)^{\frac{1}{2}}x}{n-1}\right]. \qquad (12)$$

From Eq. (12) we see that V_0 is a periodic function of x if $\lambda_0>0$, while $V_0\equiv 0$, if $\lambda_0=0$. Since the integral in Eq. (2) would not exist, if V_0 were periodic, and no eigenvalues would exist, if $V_0\equiv 0$, we conclude that $\lambda_0<0$. Then Eq. (12) shows that V_0 vanishes as $|x|$ becomes infinite. Since u_0 must also vanish at infinity, we see from Eq. (6) that $n>1$.

Now Eqs. (12) and (2) yield a relation among λ_0, n, and k which is

$$\left(\frac{-n\lambda_0}{n-1}\right)^n \frac{2(n-1)}{(-\lambda_0)^{\frac{1}{2}}} \int_0^{\infty} \text{sech}^{2n}y\,dy = k. \qquad (13)$$

Since $n>1$ and $\lambda_0>0$, we see from Eq. (13) that $k>0$. The integral in Eq. (13) has the value[4]

$$\int_0^{\infty} \text{sech}^{2n}y\,dy = \frac{\Gamma(n)\Gamma(\frac{1}{2})}{2\Gamma(n+\frac{1}{2})}. \qquad (14)$$

By using Eq. (14) in Eq. (13) and solving for λ_0, we obtain

$$-\lambda_0 = -F(n)k^{2/2n-1}. \qquad (15)$$

Here $F(n)$ is given by

$$F(n) = \left[\frac{\Gamma(n+\frac{1}{2})}{(n-1)\pi^{\frac{1}{2}}\Gamma(n)}\left(\frac{n-1}{n}\right)^n\right]^{2/2n-1}. \qquad (16)$$

[4] W. Grobner and N. Hofreiter, *Integraltafel* (Springer-Verlag, Berlin, Germany, 1949), Chap. II, p. 162, Eq. (12).

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We have now found that for any $k>0$ and any $n>1$ there is exactly one potential $V_0(x)$ given by Eq. (12), with λ_0 given by Eq. (15), which renders stationary an eigenvalue of Eq. (1). There is no such potential, if $k\leqq 0$ or $n\leqq 1$. The corresponding eigenfunction u_0 is, from Eqs. (6) and (12),

$$u_0(x)=\left\{\frac{-\lambda_0 n}{n-1}\operatorname{sech}^2\left[\frac{(-\lambda_0)^{\frac{1}{2}}x}{n-1}\right]\right\}^{(n-1)/2} \quad (17)$$

Since $u_0(x)\neq 0$, λ_0 is the lowest eigenvalue of the potential $V_0(x)$.

3. ISOPERIMETRIC INEQUALITIES AND LOWER BOUNDS

Let us now assume that the stationary value λ_0 is actually the minimum value of the lowest eigenvalue of any potential satisfying Eq. (2), which we shall prove in the next section. Then, if λ is the lowest eigenvalue of some potential $V(x)$, we have $\lambda\geqq\lambda_0$ provided $V(x)$ satisfies Eq. (2). If we define k in terms of $V(x)$ by Eq. (2), and use Eq. (15) for λ_0 we then have the inequality

$$\lambda\geqq -F(n)\left[\int_{-\infty}^{\infty}V^n(x)dx\right]^{2/(2n-1)}. \quad (18)$$

Equality holds in Eq. (18) only if $V(x)=V_0(x)$. For each $n>1$ this inequality (18) is the isoperimetric inequality we sought. It provides lower bounds on the lowest eigenvalue λ. A graph of $F(n)$ is shown in Fig. 1.

In the limit $n=1$, Eq. (18) yields the following lower bound, obtained previously by Larry Spruch:

$$\lambda\geqq -\tfrac{1}{4}\left[\int_{-\infty}^{\infty}V(x)dx\right]^2. \quad (19)$$

As n tends to unity, the limiting form of the potential $V_0(x)$, given by Eq. (12), is the delta function for which equality holds in Eq. (19).

To illustrate the use of Eq. (18), we shall now apply it to a square well of depth V and width $2a$. The

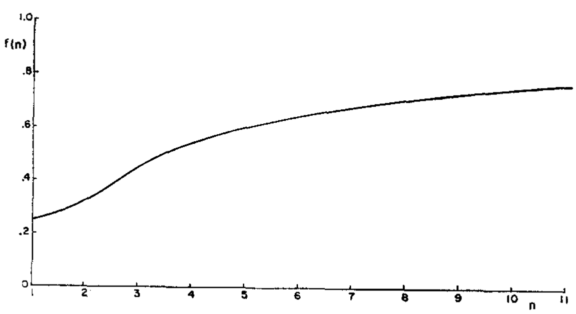

FIG. 1. The function $F(n)$, given by Eq. (16), as a function of n. This function occurs in the isoperimetric inequality (18). As n becomes infinite, $F(n)$ approaches unity.

integral in Eq. (18) is then $2aV^n$ and Eq. (18) becomes

$$\lambda/V\geqq -F(n)(4a^2V)^{1/2n-1}. \quad (20)$$

A simple calculation shows that the right-hand side of Eq. (20) is largest when n satisfies the equation

$$4a^2V=\pi n(n-1)\frac{\Gamma^2(n)}{\Gamma^2(n+\frac{1}{2})}\times\exp\{(2n-1)[\Psi(n+\tfrac{1}{2})-\Psi(n)]\}. \quad (21)$$

Here $\Psi(n)=\Gamma'(n)/\Gamma(n)$. A graph of the lower bound Eq. (20) with n determined from Eq. (21) is shown in Fig. 2 as a function of a^2V. For comparison the exact value of λ is also shown.

Let us now apply Eq. (18) to the exponential potential of depth V and range a given by

$$V(x)=Ve^{-|x|/a}. \quad (22)$$

Upon inserting Eq. (22) into Eq. (18), we obtain

$$\lambda/V\geqq -F(n)(4a^2V/n^2)^{1/(2n-1)}. \quad (23)$$

The right-hand side of Eq. (23) is largest when n

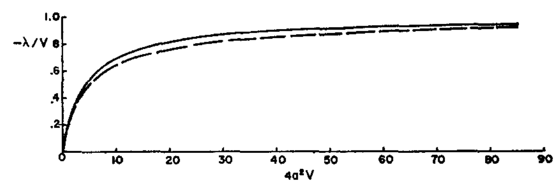

FIG. 2. The best lower bound on the lowest eigenvalue of a square well potential of depth V and width $2a$ is shown as a function of a^2V (solid curve). The exact lowest eigenvalue is also shown for comparison (dashed curve). The ordinate is $-\lambda/V$, and the bound is computed from Eqs. (20) and (21).

satisfies the equation

$$4a^2V=\pi n^3(n-1)\frac{\Gamma^2(n)}{\Gamma^2(n+\frac{1}{2})}\times\exp\{(2n-1)[\Psi(n+\tfrac{1}{2})-\Psi(n)-1/n]\}. \quad (24)$$

The lower bound on λ/V given by Eq. (23), with n determined by Eq. (24), is shown in Fig. 3 as a function of a^2V.

As another example of the use of Eq. (18), let us apply it to the inverse αth power potential of depth V and range a given by

$$V(x)=V/(1+a^{-1}|x|)^{\alpha}. \quad (25)$$

For this potential Eq. (18) yields

$$\lambda/V\geqq -F(n)[4a^2V/(n\alpha-1)^2]^{1/(2n-1)}. \quad (26)$$

The bound in Eq. (26) is largest when n satisfies the equation

$$4a^2V=\pi n(n-1)(n\alpha-1)^2[\Gamma^2(n)/\Gamma^2(n+1/2)]\times\exp\{(2n-1)[\Psi(n+\tfrac{1}{2})-\Psi(n)-\alpha/(n-1)]\}. \quad (27)$$

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4. PROOF THAT λ_0 IS A MINIMUM

To prove that λ_0 is the minimum value of the lowest eigenvalue of any potential satisfying Eq. (2), we begin with the variational characterization of the lowest eigenvalue of a potential $V(x)$. It is

$$\lambda=\min_v\left[\int_{-\infty}^{\infty}(v_x^2-v^2V)dx\Big/\int_{-\infty}^{\infty}v^2dx\right]. \qquad (28)$$

Following a suggestion of H. F. Weinberger, we make use of the Holder inequality which holds for any $n>1$

$$\int_{-\infty}^{\infty}v^2Vdx\leqq\left(\int_{-\infty}^{\infty}V^ndx\right)^{1/n}\left(\int_{-\infty}^{\infty}v^{2n/n-1}dx\right)^{(n-1)/n}. \qquad (29)$$

Equality obtains in Eq. (29) if and only if $V^{n-1}=v^2$, which is the same condition as Eq. (6). Upon inserting Eq. (29) into Eq. (28), and making use of Eq. (2), we obtain

$$\lambda\geqq\min_v\left[\int_{-\infty}^{\infty}v_x^2dx-k^{1/n}\left(\int_{-\infty}^{\infty}v^{2n/(n-1)}dx\right)^{(n-1)/n}\Big/\int_{-\infty}^{\infty}v^2dx\right]. \qquad (30)$$

We must now show that the right-hand side of Eq. (30) is minimized when $v=v_0$. If it is, then the right side of Eq. (30) is just λ_0 since for v_0 and V_0 equality holds in Eq. (29), and, therefore, in Eq. (30). Then Eq. (30) yields the desired inequality

$$\lambda\geqq\lambda_0. \qquad (31)$$

A necessary condition for v to minimize the expression on the right-hand side of Eq. (30) is obtained by requiring the first variation of that expression to vanish. This yields the condition

$$v_{xx}+k^{1/n}\left(\int_{-\infty}^{\infty}v^{2n/(n-1)}dx\right)^{-1/n}v^{1+(2/n-1)}+\lambda'v=0. \qquad (32)$$

Here λ' denotes the minimum value of the expression on the right-hand side in Eq. (30). This equation becomes identical with Eq. (7), if we introduce $x'=cx$ and $\lambda''=c^{-2}\lambda'$ where

$$c^2=k^{1/n}\left(\int_{-\infty}^{\infty}v^{2n/(n-1)}dx\right)^{-1/n}. \qquad (33)$$

Therefore, its solution is just $c^{1-n}u_0(x)$, as we see from Eq. (17), with λ' in place of λ_0. Then Eq. (33), which determines λ', becomes identical with Eq. (13) so $\lambda'=\lambda_0$. Therefore, if the minimum in Eq. (30) exists, its value is λ_0 and the minimizing function is $v_0(x)$.

The existence of the minimum in Eq. (30) can be proved by standard methods of the calculus of variations, although the proof is by no means trivial.

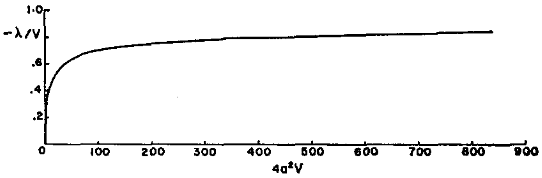

FIG. 3. The best lower bound on the lowest eigenvalue of the exponential potential $V(x)=V\exp(-|x|/a)$ of depth V and range a is shown as a function of a^2V. The ordinate is $-\lambda/V$ and the bound is computed from Eqs. (23) and (24).

5. AN UPPER BOUND

Let us now consider the isoperimetric problem obtained by replacing the class of potentials satisfying Eq. (2) by those satisfying the condition

$$\int_{-\infty}^{\infty}V(x)\rho^2(x)dx=k. \qquad (2')$$

Here $\rho(x)$ is a given function and k is a given constant. By proceeding as in Sec. 2 we obtain, instead of Eq. (4),

$$\int_{-\infty}^{\infty}\dot{V}\rho^2dx=0. \qquad (4')$$

Then instead of Eq. (6), we find from Eqs. (4′) and (5) $u_0^2=\rho^0$ or equivalently

$$u_0(x)=\rho(x). \qquad (6')$$

Since u_0 is quadratically integrable, we see that $\rho(x)$ must also be so. Now Eqs. (1) and (6′) yield

$$V_0(x)=-\lambda_0-\rho^{-1}\rho_{xx}. \qquad (12')$$

From Eq. (2′) and (12′) we find λ_0 which is given by

$$\lambda_0=\left(\int_{-\infty}^{\infty}\rho_x^2dx-k\right)\Big/\int_{\infty}^{\infty}\rho^2dx. \qquad (15')$$

If λ_0 is the maximal lowest eigenvalue of any potential satisfying Eq. (2′), then $\lambda\leqq\lambda_0$, or using Eqs. (15′) and (2′),

$$\lambda\leqq\left(\int_{-\infty}^{\infty}\rho_x^2dx-\int_{-\infty}^{\infty}\rho^2Vdx\right)\Big/\int_{-\infty}^{\infty}\rho^2dx. \qquad (16')$$

But Eq. (16′) is true, since the right-hand side is just the Rayleigh quotient evaluated for the trial function $\rho(x)$. Thus we have found that this Rayleigh quotient is the largest lowest eigenvalue of any potential satisfying Eq. (2′) and it is attained for the potential in Eq. (12′).

6. HIGHER DIMENSIONS

Some of the preceding considerations apply in any number of dimensions. Even many of our equations remain valid, if we interpret x as a vector and replace u_{xx} by ∇^2u. With these changes Eqs. (1)–(7) remain valid. Then Eq. (7) is the equation which must be

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satisfied by the eigenfunction u_0 of the potential V_0 which makes λ stationary. If we seek a spherically symmetric solution $u_0(r)$, then Eq. (7) becomes, in three dimensions,

$$u_{0rr}+(2/r)u_{0r}+u_0^{1+(2/n-1)}+\lambda_0 u_0=0. \qquad (7'')$$

It has not been possible to solve this equation explicitly.

All of the equations of Sec. 4 remain valid, if we also replace v_x^2 by $(\nabla v)^2$. However, the proof of the existence of the minimum in Eq. (30) has not been carried out, nor has it been shown that the minimizing potential, if one exists, is spherically symmetric.

All the results of Sec. 5 hold in any number of dimensions.

Errata: Statistical Dynamics of Simple Cubic Lattices. Model for the Study of Brownian Motion

[J. Math. Phys. 1, 309 (1960)]

Robert J. Rubin
National Bureau of Standards, Washington 25, D. C.

In Eqs. (16), (17), (19), (A1), and in the integral at the end of Sec. III (p. 312), replace **V** by $-$**V** where it appears explicitly. In the fourth and fifth lines following Eq. (16), delete the expression in brackets.

In Eq. (7a), replace $(2N+1)^{-n/2}$ by $(2N+1)^{-n}$.

In Eq. (C2), replace $\ln(\frac{1}{2}\rho^2)$ by $\ln(1/2\rho^2)$.

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