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LOWER BOUNDS FOR THE INFIMUM OF THE SPECTRUM OF THE SCHRÖDINGER OPERATOR IN $\mathbb{R}^N$ AND THE SOBOLEV INEQUALITIES

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Abstract

This article is concerned with the infimum e_1 of the spectrum of the Schrödinger operator $\tau = -\Delta + q$ in $\mathbb{R}^N$, $N \geq 1$. It is assumed that $q_- = \max(0, -q) \in L^p(\mathbb{R}^N)$, where $p \geq 1$ if $N = 1$, $p > N/2$ if $N \geq 2$. The infimum e_1 is estimated in terms of the L^p-norm of q_- and the infimum $\lambda_{N,\theta}$ of a functional $\Lambda_{N,\theta}(\nu) = \|\nabla v\|_2^\theta \|v\|_2^{1-\theta} \|v\|_r^{-1}$, with ν element of the Sobolev space $H^1(\mathbb{R}^N)$, where $\theta = N/(2p)$ and $r = 2N/(N-2\theta)$. The result is optimal. The constant $\lambda_{N,\theta}$ is known explicitly for $N = 1$; for $N \geq 2$, it is estimated by the optimal constant $C_{N,s}$ in the Sobolev inequality, where $s = 2\theta = N/p$. A combination of these results gives an explicit lower bound for the infimum e_1 of the spectrum. The results improve and generalize those of Thirring [*A Course in Mathematical Physics III. Quantum Mechanics of Atoms and Molecules*, Springer, New York 1981] and Rosen [*Phys. Rev. Lett.*, **49** (1982), 1885-1887] who considered the special case $N = 3$. The infimum $\lambda_{N,\theta}$ of the functional $\Lambda_{N,\theta}$ is calculated numerically (for $N = 2, 3, 4, 5$, and 10) and compared with the lower bounds as found in this article. Also, the results are compared with these by Nasibov [*Soviet. Math. Dokl.*, **40** (1990), 110-115].

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Key words: Optimal lower bound, infimum spectrum Schrődinger operator, Sobolev inequality

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1. Results

In this article we study the Schrödinger operator $\tau = -\Delta + q$ on $\mathbb{R}^N$. The real-valued potential q is such that $q = q_+ + q_-$, where

$$q_+ = \max(0, q) \in L^2_{loc}(\mathbb{R}^N), \tag{1.1}$$

$$q_- = \max(0, -q) \in L^p(\mathbb{R}^N), \quad \begin{array}{ll} N = 1: & 1 \leq p < \infty, \\ N \geq 2: & N/2 < p < \infty. \end{array} \tag{1.2}$$

Associated with q is the closed hermitian form h,

$$h(u, v) = (\nabla u, \overline{\nabla v}) + \int_{\mathbb{R}^N} q u \bar{v} dx, \qquad u, v \in Q(h), \tag{1.3}$$

$$Q(h) = H^1(\mathbb{R}^N) \cap \{u \mid u \in L^2(\mathbb{R}^N), \quad q_+^{1/2} \in L^2(\mathbb{R}^N)\}. \tag{1.4}$$

As will be shown in the course of the proof of Theorem 1.1, h is semibounded below if the condition (1.2) is satisfied. Hence, we can define a unique self-adjoint operator H, such that $Q(h)$ is its quadratic form (see [22, Theorem VIII.15] or [26, Theorem 2.5.19]).

We remark that τ restricted to $C_0^\infty(\mathbb{R}^N)$ is essentially self-adjoint for the following values of p :

$$\begin{array}{ll} p \geq 2 & \text{if } N = 1, 2, 3; \\ p > 2 & \text{if } N = 4; \\ p \geq N/2 & \text{if } N \geq 5; \end{array} \tag{1.5}$$

see [21, Corollary, p. 199, with $V_1 = q_+$, $c = d = 0$, $V_2 = q_-$]. For $N = 1, 2, 3$ condition (1.5) imposes a restriction on the values of p allowed in (1.2). Furthermore, $\mathcal{D}(H) = H_0^2(\mathbb{R}^N) = H^2(\mathbb{R}^N)$ if $q_+ \in L^\infty(\mathbb{R}^N)$, $p > N/2$, $N \geq 4$; see [6, pp. 123, 246 (vi)].

It is our purpose to give a lower bound for the infimum of the spectrum of H by estimating the Rayleigh quotient $e_1 = \inf_{u \in \mathcal{D}(H)} h(u,u)/\|u\|_2^2$. Since q_+ enlarges e_1, it suffices to consider the Rayleigh quotient for the case $q_+ = 0$.

Let $\Lambda_{N,\theta}$ be the following functional on $H^1(\mathbb{R}^N)$:

$$\Lambda_{N,\theta}(v) = \frac{\|\nabla v\|_2^\theta \|v\|_2^{1-\theta}}{\|v\|_r}, \quad r = 2N/(N - 2\theta), \quad v \in H^1(\mathbb{R}^N), \tag{1.6}$$

where

$$0 < \theta \leq 1/2 \text{ if } N = 1, \qquad \text{and} \qquad 0 < \theta < 1 \text{ if } N \geq 2.$$

Let $\lambda_{N,\theta}$ be its infimum

$$\lambda_{N,\theta} = \inf \left\{ \Lambda_{N,\theta}(v) | v \in H^1(\mathbb{R}^N),\ v \neq 0 \right\}. \tag{1.7}$$

It is possible to include the cases $\theta = 0$, with $\lambda_{N,0} = \Lambda_{N,0}(v) = 1$, and $\theta = 1$, provided $N \geq 2$; see below. The functional $\Lambda_{N,\theta}(v)$ is invariant for dilations in the argument of v and for scaling of v.

We recall the following imbeddings

$$H^1(\mathbb{R}^1) \hookrightarrow C^{0,\lambda}(\overline{\mathbb{R}^1}),\ 0 < \lambda \leq 1/2, \tag{1.8}$$

$$H^1(\mathbb{R}^2) \hookrightarrow L^s(\mathbb{R}^2),\ 2 \leq s < \infty, \tag{1.9}$$

$$H^1(\mathbb{R}^N) \hookrightarrow L^s(\mathbb{R}^N),\ 2 \leq s \leq 2N/(N-2),\ N \geq 3; \tag{1.10}$$

see [1, pp. 97, 98]. Here, $C^{0,\lambda}(\overline{\mathbb{R}^1})$ is the space of bounded, uniformly continuous functions v on $\mathbb{R}^1$ with

$$\sup_{x,y\in\mathbb{R}^1,\ x\neq y} |v(x)-v(y)|/|x-y|^\lambda < \infty.$$

Hence, $u \in H^1(\mathbb{R}^1)$ implies $u \in L^2(\mathbb{R}^1)\cap L^\infty(\mathbb{R}^1)$ and, therefore, $u \in L^s(\mathbb{R}^1)$, $2 \leq s \leq \infty$. Thus, (1.8), (1.9), and (1.10) imply that there exist positive constants K such that

$$[\|\nabla v\|_2^2 + \|v\|_2^2]^{1/2}/\|v\|_s \geq K, \qquad \begin{array}{c} 2 \leq s \leq \infty \text{ if } N = 1, \\ 2 \leq s < \infty \text{ if } N = 2, \\ 2 \leq s \leq 2N/(N-2) \text{ if } N \geq 3. \end{array} \tag{1.11}$$

Returning to the functional $\Lambda_{N,\theta}$, we make for $0 < \theta < 1$ ($0 < \theta \leq 1/2$ if $N = 1$) a dilation $x = \epsilon y$, $x, y \in \mathbb{R}^N$, $w(y) = v(x)$, such that

$$\|\nabla w\|_2^2/\|w\|_2^2 = \theta/(1-\theta).$$

The inequality

$$ab \leq a^P/P + b^Q/Q,\ a,b \geq 0,\ 1 < P < \infty,\ 1/P + 1/Q = 1, \tag{1.12}$$

with equality if and only if $a^P = b^Q$, applied to $\Lambda^2_{N,\theta}(w)$ gives ($P = 1/\theta$, $Q = 1/(1-\theta)$, $a = \eta\|\nabla w\|_2^{2\theta}$, $b = \|w\|_2^{2\theta}/\eta$)

$$\Lambda^2_{N,\theta}(w) \leq \frac{\theta\eta^{1/\theta}\|\nabla w\|_2^2 + (1-\theta)\eta^{-1/(1-\theta)}\|w\|_2^2}{\|w\|_r^2}, \tag{1.13}$$

for some number $\eta > 0$. Equality holds if and only if

$$\eta^{1/\theta}\|\nabla w\|_2^2 = \eta^{-1/(1-\theta)}\|w\|_2^2, \quad \text{i.e. } \eta^{-1/(\theta(1-\theta))} = \theta/(1-\theta).$$

In this case,

$$\Lambda_{N,\theta}^2(w) = \theta^\theta(1-\theta)^{1-\theta}\frac{\|\nabla w\|_2^2 + \|w\|_2^2}{\|w\|_r^2}. \tag{1.14}$$

Since it is possible to perform this dilation for any $v \in H^1(\mathbb{R}^N)$, and since $\theta^\theta (1-\theta)^{1-\theta} > 0$ we conclude that $\lambda_{N,\theta} > 0$ for $0 < \theta < 1$. The case $N = 1$, $\theta = 1/2$ (in that case r becomes undefined) is covered by the value $s = \infty$ in (1.11). The cases $\theta = 1$, $N \geq 2$ are covered by a special form of the Sobolev inequality

$$\|\nabla w\|_s \geq C_{N,s}\|w\|_t,\ t = sN/(N-s),\ 1 \leq s < N,\ w \in H^{1,s}(\mathbb{R}^N), \tag{1.15}$$

where $C_{N,s}$ are the optimal constants and

$$\begin{aligned} &H^{1,s}(\mathbb{R}^N) \\ &\quad = \text{completion of } \{w \mid w \in C^1(\mathbb{R}^N), \|u\|_{1,s}^s = \|u\|_s^s + \|\nabla u\|_s^s < \infty\} \\ &\quad\quad \text{with respect to the norm } \|\cdot\|_{1,s}. \end{aligned} \tag{1.16}$$

If we take $s = 2$ we have $\lambda_{N,1} = C_{N,2}$, $N \geq 3$. Since $H^1(\mathbb{R}^2) \not\hookrightarrow L^\infty(\mathbb{R}^2)$, it follows that $\lambda_{2,1} = C_{2,2} = 0$, *i.e.* $K = 0$ in (1.11). The numbers $C_{N,s}$ are known explicitly by the work of [2] and [25], see also [14]

$$C_{N,s} = N^{1/s}\left(\frac{N-s}{s-1}\right)^{(s-1)/s} \times\left[N\omega_N B\left(\frac{N}{s}, N+1-\frac{N}{s}\right)\right]^{1/N}, \; 1<s<N, \tag{1.17}$$

$$C_{N,1} = N\omega_N^{1/N}, \; N \geq 2, \tag{1.18}$$

where ω_N is the volume of the unit ball in $\mathbb{R}^N$:

$$\omega_N = \pi^{N/2}/\Gamma(1+N/2), \tag{1.19}$$

$$B(a,b) = \Gamma(a)\Gamma(b)/\Gamma(a+b), \; a,b>0, \tag{1.20}$$

and there is equality in (1.15) for functions of the form

$$w_{N,s}(x_1,...,x_N) = \left\{a+b|x|^{s/(s-1)}\right\}^{1-N/s}, \; a,b>0, \; 1<s<N. \tag{1.21}$$

Note that $w_{N,s} \notin L^s(\mathbb{R}^N)$ if $s \geq N^{1/2}$. For $s=1$ there are no functions such that there is equality, but by taking an approximating sequence $\{w^i\} \in H^{1,1}(\mathbb{R}^N)$ of the characteristic function of the unit ball, the bound $C_{N,1}$ can be approximated arbitrarily close. See further Lemma 2.1 for more information about $\Lambda_{N,\theta}$ and the explicit form for $\lambda_{1,\theta}$.

In Theorem 1.1 we give the lowest possible point of the spectrum of this Schrödinger equation for all q_- satisfying (1.2). Let us define the number

$l(N,\theta)$, where $\theta = N/(2p)$, as follows

$$l(N,\theta) = \inf_{q_- \in L^p(\mathbb{R}^N)} \inf_{u \in H^1(\mathbb{R}^N)} \frac{\|\nabla u\|_2^2 + \int_{\mathbb{R}^N} q\|u\|_2^2 dx}{\|u\|_2^2} \|q_-\|_p^{-1/(1-\theta)}. \tag{1.22}$$

Theorem 1.1. *Let $q_- \in L^p(\mathbb{R}^N)$, $1 \le p < \infty$ if $N = 1$, $N/2 < p < \infty$ if $N \ge 2$ (i.e. (1.2)). Then*

$$l(N,\theta) = -(1-\theta)\theta^{\theta/(1-\theta)}\lambda_{N,\theta}^{-2/(1-\theta)}, \quad \begin{array}{l} 0 < \theta < 1/2 \text{ if } N = 1, \\ 0 < \theta < 1 \text{ if } N \ge 2, \end{array} \tag{1.23}$$

and explicitly for $N = 1$

$$\begin{aligned} &l(1,\theta) \\ &= -\left\{(2\theta)^{2\theta}(1-2\theta)^{1-2\theta}\left[B\left(\frac{1}{2},\frac{1}{2\theta}\right)\right]^{-2\theta}\right\}^{1/(1-\theta)}, 0 < \theta < 1/2, \\ &= -\left\{p^{-p}(p-1)^{p-1}\left[B\left(\frac{1}{2},p\right)\right]^{-1}\right\}^{2/(2p-1)}, 1 < p < \infty, \end{aligned} \tag{1.24}$$

$$l(1,1/2) = -1/4. \tag{1.25}$$

Remark 1.1. *Of course, for any application of this method to find a lower bound for e_1 (the smallest eigenvalue) one can take the following infimum over the allowed set Θ of θ-values (depending on q_-).*

$$e_1 \ge -\inf_{\theta\in\Theta}(1-\theta)\theta^{\theta/(1-\theta)}\lambda_{N,\theta}^{-2/(1-\theta)}\|q_-\|_{N/(2\theta)}^{1/(1-\theta)}. \tag{1.26}$$

Remark 1.2. *Note that we do not include $\theta = 1$ in the allowed θ-range, although for $N \geq 2$ $\lambda_{N,1}$ is defined. It turns out that the method of the proof does not work in this case; it gives however a criterion such that $\sigma_d(H) = \emptyset$ ($i.e.$ there are no isolated eigenvalues), see the Remark 2.3 after the proof of Theorem 1.1.*

Remark 1.3. *It is possible to allow the case $p = \infty$, $i.e.$ $\theta = 0$, then $l(N, 0) = -1$. If $q = -\|q_-\|_\infty$ this bound is achieved arbitrarily close by a sequence of functions $\{u^i\} \in H^1(\mathbb{R}^N)$, where each u^i is a smooth approximation of the characteristic function of the i-ball in $\mathbb{R}^N$, because then the quotient*

$$\|\nabla u^i\|_2^2/\|u^i\|_2^2 \to N\omega_N i^{-1},\ i \to \infty, \quad \textit{and} \quad \frac{\int_{\mathbb{R}^N} q|u^i|^2\, dx}{\|u^i\|_2^2}\|q_-\|_\infty^{-1} = -1.$$

Remark 1.4. *Already Lieb and Thirring [15] characterize the infimum of the spectrum with a number $-(L^1_{\gamma,N})^{1/\gamma}$ (in their notation, $\gamma = p - N/2$), with $\gamma > \max(0, 1 - N/2)$, and $\gamma = 1/2$, $N = 1$. Therefore,*

$$(L^1_{\gamma,N})^{1/\gamma}\big|_{\gamma=(1-\theta)N/(2\theta)} = (1-\theta)\theta^{\theta/(1-\theta)}\lambda_{N,\theta}^{-2/(1-\theta)}. \tag{1.27}$$

They give $L^1_{\gamma,1}$ for $\gamma > 1/2$ explicitly. Here, we also include the case $N = 1$, $\gamma = 1/2$ (i.e. $\theta = 1/2$, $p = 1$). However, the main reason of this article is to show how one can give an explicit estimate for e_1 by sharp estimates of the numbers $\lambda_{N,\theta}$, $N \geq 2$, in terms of the numbers $C_{N,s}$ for some $s = s(\theta)$, see Theorems 1.2 and 1.3. For a survey for other integral inequalities results related to the infimum of the spectrum see [9] and [16].

Remark 1.5. *The results for the ordinary differential case $(N = 1, \Omega = \mathbb{R})$ are related to those for $\Omega = \mathbb{R}^+$ with either a Dirichlet or a Neumann boundary* *condition at $x = 0$ (respectively the operators T_0 and $T_{\pi/2}$ in the work of [8], [27] and [10]). In those cases there holds $1 \le p \le \infty$*

$$\inf_{q_- \in L^p(\mathbb{R}^+)} \inf_{u \in \mathcal{D}(T_0)} \frac{\|u'\|_2^2 + \int_0^\infty q|u|_2^2 dx}{\|u\|_2^2} \|q_-\|_p^{-2p/(2p-1)} = l(1, 1/(2p)), \tag{1.28}$$

$$\inf_{q_- \in L^p(\mathbb{R}^+)} \inf_{u \in \mathcal{D}(T_{\pi/2})} \frac{\|u'\|_2^2 + \int_0^\infty q|u|_2^2 dx}{\|u\|_2^2} \|q_-\|_p^{-2p/(2p-1)} = 2^{2/(2p-1)} l(1, 1/(2p)). \tag{1.29}$$

See for related work [3].

Theorem 1.2. *The following inequalities hold for $N \ge 2$*

$$\text{i) } \lambda_{N,\theta} > (\lambda_{N,\theta'})^\alpha (\lambda_{N,\theta''})^{1-\alpha}, \; 0 < \alpha < 1, \quad \theta = \alpha\theta' + (1-\alpha)\theta'', \; \theta' \ne \theta'', \tag{1.30}$$

$$\text{ii) } \lambda_{N,\theta} > (\theta C_{N,2\theta})^\theta, \quad 1/2 \le \theta < 1, \tag{1.31}$$

$$\text{iii) } \lambda_{N,\theta} > (\theta_N C_{N,2\theta_N})^\theta, \quad 0 < \theta \le \theta_N, \qquad \lambda_{N,\theta} > (\theta C_{N,2\theta})^\theta, \quad \theta_N \le \theta < 1, \tag{1.32}$$

$$\text{iv) } \lambda_{N,\theta} > (C_{N,2})^\theta, \quad 0 < \theta < 1, \tag{1.33}$$

where $C_{N,s}$ is given by (1.17) and (1.18) and $\theta_N = \theta(N) \in (1/2, 1)$ is the unique maximum of $\theta C_{N,2\theta}$, $1/2 \le \theta \le 1$. θ_N is given by $\theta_N = N/(2p_N)$ where

p_N is the solution of $M(N,p)=0$, with

$$M(N,p)=\log\left(\frac{N-p}{p-1}\right)+\frac{N-p}{p(p-1)}+\psi(p)-\psi(N+1-p), \tag{1.34}$$

$$\psi(x)=\frac{d}{dx}(\log(\Gamma(x))=\left(\frac{d}{dx}\Gamma(x)\right)/\Gamma(x), \quad x>0. \tag{1.35}$$

It is now easy to combine both theorems in

Theorem 1.3. *Under the conditions of Theorem 1.1 there holds*

$$l(N,\theta)>\begin{cases}-(1-\theta)\theta^{\theta/(1-\theta)}(\theta_N C_{N,2\theta_N})^{-2\theta/(1-\theta)}, & 0<\theta\le\theta_N,\\ -(1-\theta)\theta^{-\theta/(1-\theta)}(C_{N,2\theta})^{-2\theta/(1-\theta)}, & \theta_N\le\theta<1,\end{cases} \tag{1.36}$$

and also (generally less than optimal)

$$l(N,\theta)>-(1-\theta)\theta^{\theta/(1-\theta)}(\theta' C_{N,2\theta'})^{-2\theta/(1-\theta)}, \quad 0<\theta<1,\ \text{for any } \theta'\ge\theta,\ 1/2\le\theta'\le 1. \tag{1.37}$$

Proof. Equation (1.36) follows from (1.23) and (1.32); (1.37) follows from (1.23), (1.30) (with $\theta''=0$) and (1.31). □

Remark 1.6. *For $N=3$, $\theta'=1$ the result (1.37) reads explicitly*

$$l(3,\theta)>-(1-\theta)\theta^{\theta/(1-\theta)}[3^{1/2}2^{-2/3}\pi^{2/3}]^{-2\theta/(1-\theta)}, \quad 0<\theta<1, \tag{1.38}$$

and this is the same result as [23, (14)].

Remark 1.7. *[26, (3.5.30), and private communication by H. Grosse] gives the following result for* $N = 3$

$$l(3,3/(2p)) > -((p-1)/p)^2(4\pi)^{-2/(2p-3)} \times \left[\Gamma\left(\frac{2p-3}{p-1}\right)\right]^{(2p-2)/(2p-3)}, \quad 3/2 < p < \infty, \tag{1.39}$$

or in terms of θ,

$$l(3,\theta) > -(1-2\theta/3)^2(4\pi)^{-2\theta/(3-3\theta)} \times \left[\Gamma\left(\frac{6-6\theta}{3-2\theta}\right)\right]^{(3-2\theta)/(3-3\theta)}, \quad 0 < \theta < 1. \tag{1.40}$$

It can be proved that (1.38) is better than (1.40) for all $0 < \theta < 1$*. For* $\theta = 0$ *the right-hand sides of both (1.38) and (1.40) give the correct value* $l(3,0) = -1$.

Remark 1.8. *To show the superiority of (1.37) with* $\theta' < 1$ *against (1.37) with* $\theta' = 1$, $i.e.$ *(1.38), we evaluate the bound for* $l(3,3/4)$ *of (1.37) with* $\theta = \theta' = 3/4$*. We find*

$$l(3,3/4) > -2^2 3^{-7}\pi^{-2} \simeq -1.85_{10^{-4}}, \tag{1.41}$$

while (1.38) gives

$$l(3,3/4) > -2^{-4}\pi^{-4} \simeq -6.42_{10^{-4}},$$

and (1.40) gives

$$l(3,3/4) > -2^{-6}\pi^{-2} \simeq -15.83_{10^{-4}}.$$

Based on our numerical calculations (see Section 3) we find $l(3,3/4) = -1.750180_{10^{-4}}$. *So the estimate (1.41) comes close to the actual value of* $l(3,3/4)$.

Remark 1.9. *The results in Theorems 1.1, 1.2, and 1.3 were announced in [28] and [7, p. 337].*

Remark 1.10. *In the interesting paper [20] Nasibov has given a lower bound (in his notation* $1/\overline{k_0}$*) for* $\lambda_{N,\theta}$*:*

$$\lambda_{N,\theta} = \frac{1}{k_0} > \frac{1}{\overline{\overline{k_0}}}, \tag{1.42}$$

with

$$\overline{k_0} = \frac{1}{\sqrt{\theta^\theta (1-\theta)^{1-\theta}}} \left(N\omega_N B\left(\frac{N}{2}, \frac{N(1-\theta)}{2\theta}\right)\right)^{\theta/N} \times k_B\left(\frac{2N}{N+2\theta}\right), \tag{1.43}$$

$$k_B(p) = \left[\left(\frac{p}{2\pi}\right)^{1/p}\left(\frac{p'}{2\pi}\right)^{-1/p'}\right]^{N/2}, \qquad \frac{1}{p}+\frac{1}{p'} = 1. \tag{1.44}$$

And, even better

$$\lambda_{N,\theta} = \frac{1}{k_0} > \frac{1}{\overline{\overline{\overline{k_0}}}}, \qquad \textit{with} \quad \frac{1}{\overline{\overline{\overline{k_0}}}} > \frac{1}{\overline{\overline{k_0}}}, \quad \textit{for} \quad \theta > N/4, \tag{1.45}$$

with

$$\overline{\overline{k_0}} = \left\{ \frac{1}{\theta^\theta (1-\theta)^{1-\theta}} k_B \left(\frac{N}{N-2\theta} \right) \times k_B^2 \left(\frac{2N}{N+2\theta} \right) \|G(|x|)\|_{\frac{N}{N-2\theta}} \right\}^{1/2}, \tag{1.46}$$

$$G(|x|) = K_{\frac{N-2}{2}}(|x|)|x|^{-(N-2)/2}, \tag{1.47}$$

with K_α *the modified Bessel function of the second kind and order* α. *The inequality (1.45) is only relevant for* $N = 2$, $1/2 \le \theta \le 1$, *and* $N = 3$, $3/4 \le \theta \le 1$, *since* $\overline{k_0} < \overline{\overline{k_0}}$, *for* $N = 2, 0 < \theta < 1/2$, *and* $N = 3, 0 < \theta < 3/4$, *and* $\overline{k_0} = \overline{\overline{k_0}}$, *for* $N = 2$, $\theta = 1/2$, *and* $N = 3$, $\theta = 3/4$.

The reader is advised to consult also the original paper (*Dokl. Akad. Nauk SSSR* 307, No. 3, 538-542 (1989)) of [20] since there are a number of misprints in the translated version. In Section 3 this lower bound will be compared with (1.32). The function G reads

$$N = 2, \qquad G(|x|) = K_0(|x|),$$

$$N = 3, \qquad G(|x|) = K_{\frac{1}{2}}(|x|)|x|^{-1/2} = \sqrt{\frac{\pi}{2}} \exp(-|x|)/|x|,$$

so, one has to calculate the integrals in (1.46)

$$N = 2 : \|G(|x|)\|_{\frac{1}{1-\theta}} = \left[\int_0^\infty K_0^{1/(1-\theta)}(r)\, 2\pi r\, dr \right]^{1-\theta}, \tag{1.48}$$

$$N = 3 : \|G(|x|)\|_{\frac{3}{3-2\theta}} = \sqrt{\frac{\pi}{2}} \left[\int_0^\infty r^{(3-4\theta)/(3-2\theta)} \exp\left(-\frac{3r}{3-2\theta} \right) 4\pi \, dr \right]^{(3-2\theta)/3} . \tag{1.49}$$

For $N = 3$ the integral in (1.49) can be evaluated explicitly, while for $N = 2$, i.e. (1.48), that is only possible for $\theta = 1/2$:

$$\begin{aligned} N = 2 : \|G(|x|)\|_2 &= \left[2\pi \int_0^\infty K_0^2(r) \, r \, dr \right]^{1/2} \\ &= \left(2\pi \left[\frac{r^2}{2} \left(K_0^2(r) - K_1^2(r) \right) \right] \Big|_0^\infty \right)^{1/2} = \sqrt{\pi}, \end{aligned}$$

$$\begin{aligned} N = 3 : \|G(|x|)\|_{\frac{3}{3-2\theta}} \\ = \sqrt{\frac{\pi}{2}} (4\pi)^{(3-2\theta)/3} \left(\frac{3-2\theta}{3} \right)^{2-2\theta} \left[\Gamma\left(\frac{6-6\theta}{3-2\theta} \right) \right]^{(3-2\theta)/3} . \end{aligned}$$

2. Proofs

Firstly, we give more information on $\Lambda_{N,\theta}$ in a lemma.

Lemma 2.1. *The value* $\lambda_{N,\theta} = \inf_{v \in H^1(\mathbb{R}^N),\, v \neq 0} \Lambda_{N,\theta}(v)$ *for the functional* $\Lambda_{N,\theta}(v)$ *defined in (6) is attained by radial symmetric monotonely decreasing positive functions* $v_{N,\theta}(|x|)$ *which satisfy, except for* $\theta = 1/2$, $N = 1$, *the following ordinary differential equation for* $0 < \theta < 1/2$ *if* $N = 1$, *and* $0 < \theta < 1$ *if* $N \geq 2$,

$$-\frac{d^2}{dr^2}v - \frac{(N-1)}{r}\frac{d}{dr}v - v|v|^{(N+2\theta)/(N-2\theta)-1} + v = 0, \;\; r = |x| > 0,$$

$$\frac{d}{dr}v(0) = 0, \;\; \lim_{r\to\infty} v(r) = 0, \tag{2.1}$$

and the value $\lambda_{N,\theta}$ *is then given by*

$$\lambda_{N,\theta} = \theta^{\theta/2}(1-\theta)^{(N(1-\theta)-2\theta)/(2N)}\left[N\omega_N \int_0^\infty v_{N,\theta}^2(r) r^{N-1} dr\right]^{\theta/N} \tag{2.2}$$

$$\text{for} \quad 0 < \theta < 1, \quad N \geq 2.$$

For $N = 1$ *we have explicitly for* $x \geq 0$

$$v_{1,\theta}(x) = v_{1,\theta}(-x), \; 0 < \theta \leq 1/2, \tag{2.3}$$

$$v_{1,\theta}(x) = \left\{(1-2\theta)^{1/2}\cosh\left(\frac{2\theta}{1-2\theta}x\right)\right\}^{-(1-2\theta)/(2\theta)}, \; 0 < \theta < 1/2,$$

$$v_{1,1/2}(x) = e^{-x}, \tag{2.4}$$

$$\lambda_{1,\theta} = 2^{-\theta}\theta^{-\theta/2}(1-\theta)^{(1-\theta)/2}(1-2\theta)^{-(1-2\theta)/2}\left\{B\left(\frac{1}{2},\frac{1}{2\theta}\right)\right\}^{\theta}, \quad 0<\theta<1/2, \tag{2.5}$$

$$\lambda_{1,N/(2p)} = 2^{-1/2}\left\{(2p-1)^{(2p-1)/2}(p-1)^{-(p-1)}B\left(\frac{1}{2},p\right)\right\}^{1/(2p)}, \quad 1<p<\infty, \tag{2.6}$$

$$\lambda_{1,1/2} = 1. \tag{2.7}$$

Proof. The case $N = 1$ was treated by [19] and the case $N \geq 2$ was given by [29] who used a rearrangement and an inequality due to Strauss to prove the compactness of the imbedding of radial symmetric functions $u \in H^1(\mathbb{R}^N)$ into $L^s(\mathbb{R}^N)$, $2 < s < \infty$ if $N = 2$, and $2 < s < 2N/(N-2)$ if $N \geq 3$ (see also (1.9), (1.10)). The Euler equation connected with the infimum of $\Lambda_{N,\theta}$ becomes

$$-\theta\|\nabla u\|_2^{-2}\Delta u + (1-\theta)\|u\|_2^{-2}u - \|u\|_r^{-r}|u|^{r-2}u = 0,\ r = \frac{2N}{N-2\theta}, \tag{2.8}$$

which can be scaled into the form (2.1) with $\lambda_{N,\theta}$ given by (2.2). The following relations between $\lambda_{N,\theta}$ and the following norms of $\bar{v}_{N,\theta}(x_1,\ldots,x_N) = v_{N,\theta}(|x|)$ hold (*cf.* [24, p. 151], where the factor "$(n-2)$" has to be skipped in the last line on that page)

$$\|\bar{v}_{N,\theta}\|_2^2 = L(1-\theta),\ \|\nabla\bar{v}_{N,\theta}\|_2^2 = L\theta,\ \|\bar{v}_{N,\theta}\|_r^r = L, \tag{2.9}$$

$$L = \theta^{-N/2}(1-\theta)^{-N(1-\theta)/(2\theta)}\lambda_{N,\theta}^{N/\theta}. \tag{2.10}$$

Since (2.1) is nonlinear the value of $v(0)$ has to be chosen properly to satisfy $\lim_{r\to\infty} v(r) = 0$. □

Remark 2.1. *We note that the existence of solutions of (2.1) has been proved by many authors: it is just the range $0 < \theta < 1$, see [17]. The uniqueness for the full θ-range has been proved by Kwong, see [11], after preliminary work by [17], and [18]. A proof based on geometrical arguments has been given by [5]. See for related work also [12].*

Remark 2.2. *Numerical information for $\lambda_{N,\theta}$ for $N = 2,3$ can be obtained from [15, Appendix], where curves for $L^1_{\gamma,N}$ (see (1.27)) are given $(0 \le \gamma \le 2.8,$ $N = 2,3)$. By (1.27) we have*

$$\lambda_{N,\theta} = \theta^{\theta/2}(1-\theta)^{(1-\theta)/2}(L^1_{\gamma,N})^{-\theta/N}, \ \gamma = N(1-\theta)/(2\theta). \tag{2.11}$$

Comparison with (2.10) learns that $L^1_{\gamma,N} = 1/L$. Besides, the following two values for $\lambda_{N,\theta}$ are known based on numerical calculations

$$\lambda^{-1}_{2,1/2} \simeq \left(\frac{1}{\pi(1.86225\cdots)}\right) \simeq 0.642988, \text{ ([29], after (I.5))} \tag{2.12}$$

$$\to \lambda_{2,1/2} \simeq 1.55524,$$

$$\lambda^{3}_{2,2/3} \simeq 4.5981, \text{ ([13], p. 185)} \tag{2.13}$$

$$\to \lambda_{2,2/3} \simeq 1.66287.$$

Proof of Theorem 1.1. We estimate $h(u,u)$, see (1.3), as follows. All integrals are over $\mathbb{R}^N$.

$$h(u,u) = \|\nabla u\|_2^2 + \int q|u|^2 dx \tag{2.14}$$

$$\geq \|\nabla u\|_2^2 - \int q_-|u|^2 dx$$

$$\geq \|\nabla u\|_2^2 - \|q_-\|_p \|u\|_r^2 \quad [r = 2p/(p-1) = 2N/(N-2\theta)] \tag{2.15}$$

$$\geq \|\nabla u\|_2^2 - \|q_-\|_p \lambda_{N,\theta}^{-2} \|\nabla u\|_2^{2\theta} \|u\|_2^{2(1-\theta)}. \tag{2.16}$$

Apply now (1.12) with

$$P = 1/\theta, \;\; a = \theta^{-\theta} \|\nabla u\|_2^{2\theta},$$

and

$$ab = \|q_-\|_p \lambda_{N,\theta}^{-2} \|\nabla u\|_2^{2\theta} \|u\|_2^{2(1-\theta)}.$$

Then

$$b = \lambda_{N,\theta}^{-2} \theta^{\theta} \|q_-\|_p \|u\|_2^{2(1-\theta)},$$

and finally we find

$$h(u,u) = -b^Q/Q = -(1-\theta)\theta^{\theta/(1-\theta)} \lambda_{N,\theta}^{-2/(1-\theta)} \|q_-\|_p^{1/(1-\theta)} \|u\|_2^2, \tag{2.17}$$

which is the bound of Theorem 1.1. To prove the optimality part we observe that in such a case we need

$$q = q_- \quad \text{by (2.14)}, \tag{2.18}$$

$$q_- = (const)|u|^{2/(p-1)} \quad \text{by (2.15)}, \tag{2.19}$$

$$u(x_1, \dots, x_N) = (const) v_{N,\theta}(|x|) \quad \text{by (2.16)}, \tag{2.20}$$

$$a^P = b^Q, \quad \text{by (2.17)}. \tag{2.21}$$

that is

$$\theta^{-1}\|\nabla u\|_2^2 = \lambda_{N,\theta}^{-2/(1-\theta)}\theta^{\theta/(1-\theta)}\|q_-\|_p^{1/(1-\theta)}\|u\|_2^2.$$

If one takes

$$u(x_1, ..., x_N) = v_{N,\theta}(|x|), \tag{2.22}$$

and

$$q(x_1, ..., x_N) = -q_-(x_1, ..., x_N) = -\left[v_{N,\theta}(|x|)\right]^{2/(p-1)}, \tag{2.23}$$

then (2.1) becomes $-\Delta u + qu = -u$; this means that the Schrödinger equation and the Euler equation for $\Lambda_{N,\theta}$ are the same if $e_1 = -1$. This is true because for these scalings the lower bound becomes:

$$\begin{aligned} -(1-\theta)\theta^{\theta/(1-\theta)}\lambda_{N,\theta}^{-2/(1-\theta)}\|q_-\|_p^{1/(1-\theta)} \\ &= -(1-\theta)\theta^{\theta/(1-\theta)}\lambda_{N,\theta}^{-2/(1-\theta)}\left[\|\bar{v}_{N,\theta}\|_r^r\right]^{2\theta/(N(1-\theta))} \quad \text{by (2.23)}, \\ &= -1 \quad \text{by (2.9), (2.10)}. \end{aligned}$$

Finally, (2.21) is implied also by (2.9) and (2.10). It means that the infimum in (1.22) over $q_- \in L^p(\mathbb{R}^N)$ is actually attained. In addition to (2.9) there holds that for q as chosen as in (2.23)

$$\|q_-\|_p^p = L. \tag{2.24}$$

Only the case $\theta = 1/2$, $N = 1$ deserves special attention since $\frac{d}{dx}v_{1,1/2}(x)$ is not continuous at $x = 0$. We take the following sequences (see [27])

$$q_j(x) = -(j+1)[\cosh(jx)]^{-2}, \; \|q_j\|_1 = 1 + 1/j, \tag{2.25}$$

$$u_j(x) = [\cosh(jx)]^{-1/j}, \tag{2.26}$$

then u_j, q_j satisfy

$$-\frac{d^2}{dx^2}u_j + q_j u_j = -u_j,$$

so

$$\frac{\|u_j'\|_2^2 + \int_{-\infty}^{\infty} q|u_j|_2^2 dx}{\|u_j\|_2^2}\|q_j\|_1^{-2} = -(1+1/j)^2/4 > -1/4 = l(1,1/2). \tag{2.27}$$

For these sequences, $j \to \infty$, the bound can be approached arbitrarily close. □

Remark 2.3. *As one can observe the proof does not work for* $\theta = 1$, *i.e.* $p = N/2$, *however, in that case we can estimate* $(N \geq 3)$

$$\begin{aligned} h(u,u) &= \|\nabla u\|_2^2 + \int q|u|^2 dx \\ &\geq \|\nabla u\|_2^2 - \int q_-|u|^2 dx \\ &\geq \|\nabla u\|_2^2 - \|q_-\|_{N/2}\|u\|_{2N/(N-2)}^2 \\ &\geq \|\nabla u\|_2^2 \left(1 - \|q_-\|_{N/2}\lambda_{N,1}^{-2}\right). \end{aligned}$$

So, if

$$\|q_-\|_{N/2} < \lambda_{N,1}^2 = C_{N,2}^2 = \pi N(N-2)[\Gamma(N/2)/\Gamma(N)]^{2/N}, \ N \geq 3, \tag{2.28}$$

it follows that $\sigma_d(H) = \emptyset$, *i.e. there are no isolated eigenvalues. This is a well-known result, see [15, (4.24)].*

Proof of Theorem 1.2. i) By the Hölder inequality we have

$$\|v\|_r < \|v\|_{r'}^{\alpha}\|v\|_{r''}^{1-\alpha}, \ 0<\alpha<1, \ 1/r = \alpha/r' + (1-\alpha)/r'', \ r' \neq r'', \tag{2.29}$$

which inequality is strict, since $r' \neq r''$. Therefore, by the conditions specified under i)

$$\begin{aligned}\Lambda_{N,\theta}(v) &= \frac{\|\nabla v\|_2^{\theta}\|v\|_2^{1-\theta}}{\|v\|_r} \\ &> \left(\frac{\|\nabla v\|_2^{\theta'}\|v\|_2^{1-\theta'}}{\|v\|_{r'}}\right)^{\alpha}\left(\frac{\|\nabla v\|_2^{\theta''}\|v\|_2^{1-\theta''}}{\|v\|_{r''}}\right)^{1-\alpha} \\ &= \Lambda_{N,\theta'}^{\alpha}(v)\Lambda_{N,\theta''}^{1-\alpha}(v),\end{aligned} \tag{2.30}$$

and we find (1.30), which is also strict, since both infima are attained.

ii) This result is given by [13, (1.5)], by making the transformation $w = v^{1/\theta}$ for $v > 0$ in (1.15) as follows

$$C_{N,s} \leq \frac{\|\nabla w\|_s}{\|w\|_t} = \frac{\|\nabla v^{1/\theta}\|_s}{\|v^{1/\theta}\|_t} = \frac{1/\theta\|v^{(1-\theta)/\theta}\nabla v\|_s}{\|v^{1/\theta}\|_t} \qquad [t = sN/(N-s)]$$

$$= \frac{1}{\theta} \frac{\left(\int (\nabla v)^s \, v^{s(1-\theta)/\theta} dx\right)^{1/s}}{\left(\int v^{t/\theta} dx\right)^{1/t}}$$ [apply Hölder inequality, $1/P + 1/Q = 1$]

$$\leq \frac{1}{\theta} \frac{\left(\int (\nabla v)^{sP} \, dx\right)^{1/(sP)} \left(\int v^{Qs(1-\theta)/\theta} dx\right)^{1/(sQ)}}{\left(\int v^{t/\theta} dx\right)^{1/t}}$$ [take $P = 2/s$, $Q = 2/(2-s)$]

$$= \frac{1}{\theta} \frac{\left(\int (\nabla v)^2 \, dx\right)^{1/2} \left(\int v^{Qs(1-\theta)/\theta} dx\right)^{(2-s)/(2s)}}{\left(\int v^{t/\theta} dx\right)^{1/t}}$$ [take $s = 2\theta$, and $r = t/\theta = 2N/(N-2\theta)$]

$$= \frac{1}{\theta} \frac{\|\nabla v\|_2 \|v\|_2^{(1-\theta)/\theta}}{\|v\|_r^{1/\theta}} = \frac{1}{\theta} \left(\Lambda_{N,\theta}(v)\right)^{1/\theta},$$

for the choice $s = 2\theta$. We have to restrict θ to the interval $1/2 \leq \theta \leq 1$ to give the right-hand side of (31) a meaning. Again, the inequality is strict since $w = v_{N,\theta}^{\theta}$ does not equal a function $w_{N,s}$ (see (1.21)), with $s = 2\theta$.

iii) Combining i) with $\theta'' = 0$ and ii) one finds

(2.31) $$\Lambda_{N,\theta} > (\theta' C_{N,2\theta'})^{\theta}, \; 0 < \theta < 1, \; \theta \leq \theta', \; 1/2 \leq \theta' < 1.$$

This motivates the determination of the maximum of $\theta C_{N,2\theta} = (N/(2p)) C_{N,N/p}$ on $1/2 \leq \theta < 1$. There holds by (1.17), (1.18)

(2.32) $$\frac{N}{2p} C_{N,N/p} = \frac{N^2}{2p} \left(\frac{p-1}{N-p}\right)^{(N-p)/N} \times \left[N\omega_N B(p, N+1-p)\right]^{1/N}, \quad 1 < p < N,$$

(2.33) $$\frac{1}{2}C_{N,1} = (N/2)\omega_N^{1/N}, \quad p = N, \quad \theta = 1/2.$$

The maximum of (2.33) is found by putting the logaritmic derivative of (2.33) with respect to p equal to zero, which is equation (1.34). It can be proven that (1.34) has a unique solution p_N, $1 < p_N < N$, because $\frac{d}{dp}M(N,p) \le 0$. For this last inequality we use the fact that $\psi'(z) < 1/z + 1/(2z^2) + 3/(4z^3)$. So, with $\theta_N = N/(2p_N)$ and for $0 < \theta \le \theta_N$, there holds $\Lambda_{N,\theta} > (\theta_N C_{N,2\theta_N})^\theta$, and for the remaining interval $\theta_N \le \theta < 1$, $\lambda_{N,\theta} > (\theta C_{N,2\theta})^\theta$.

iv) Since $\lim_{p\to N} M(N,p) = -\infty$, it follows that $\theta C_{N,2\theta} > C_{N,2}$ for θ in a neighbourhood of $\theta = 1$. So (1.33) follows from (2.31). □

Remark 2.4. *Application of Theorem 1.2 i) with $\theta'' = 0$, $\alpha = \theta/\theta'$, gives*

(2.34) $$\lambda_{N,\theta}^2 \ge \lambda_{N,\theta'}^{2\theta/\theta'}, \quad \theta' > \theta.$$

[15, (2.21)] give the inequality

(2.35) $$L^1_{\gamma,N} \le L^1_{\gamma-1,N}(\gamma/(\gamma+N/2)),\ \gamma > 2 - N/2.$$

By (1.27) this is equivalent with

(2.36) $$\lambda_{N,\theta}^2 \ge \lambda_{N,\theta'}^{2\theta/\theta'} F(\theta,\theta'),\ \theta = N/(2p), \quad \theta' = N/(2(p-1)),$$

with

$$F(\theta,\theta') = [(1-\theta)/(1-\theta')]^{\theta(1-\theta')/\theta'}\,(\theta/\theta')^\theta.$$

For $\theta' > \theta$ it will be proved that $F(\theta, \theta') < 1$, which means that i) of Theorem 1.2 (equation (2.34)) is better than (2.35). $F(\theta, \theta') < 1$ is equivalent with

$$[\theta(1-\theta')/(\theta'(1-\theta))]^{\theta'} < (1-\theta')/(1-\theta), \tag{2.37}$$

and (2.37) is true by the inequality $(1-a)^b < 1 - ab$, $0 < a < 1$, $b < 1$, where $a = (\theta' - \theta)/(\theta'(1-\theta))$, $b = \theta'$.

Remark 2.5. *To show the merits Theorem 1.2 of ii) we compare two known values for $\lambda_{N,\theta}$, see (2.12), (2.13), by the estimate (1.31)*

$$\lambda_{2,1/2} \simeq 1.55524 > 1.33134 \cdots = \pi^{1/4} = (1/2\, C_{2,1})^{1/2}, \tag{2.38}$$

$$\lambda_{2,2/3} \simeq 1.66287 > 1.63696 \cdots = (2\pi/3)^{2/3} = (2/3\, C_{2,4/3})^{2/3}. \tag{2.39}$$

Note that in the work of Levine [13, p. 183, third line] the lower bound (2.39) is not calculated correctly. The lower bound C_1 for his variable C (which is $\lambda^3_{2,2/3}$) should be $C_1 = 4\pi^2/9 \simeq 4.38649$, in stead of $C_1 = 2\pi^{3/2}/9 \simeq 1.237$ ([13, p. 183, eighth line]). This corrected value for C_1 is a much better lower bound, since numerically we found $C = \lambda^3_{2,2/3} \simeq 1.66287^3 \simeq 4.5981$. See also Section 3 and Table 1.

Remark 2.6. *Approximate solutions p_N of (1.34) for $N = 2, 3$ and $N \to \infty$ are*

$$p_2 \simeq 1.647, \;\; \theta_2 \simeq 0.6070, \tag{2.40}$$

$$p_3 \simeq 2.304, \;\; \theta_3 \simeq 0.6509, \tag{2.41}$$

$$p_N = 2N/3 + 5/18 + O(1/N),$$
$$\theta_N = 3/4 - 5/(16N) + O(1/N^2),\ N \to \infty. \tag{2.42}$$

The knowledge of (2.40) allows us to improve (2.38) as follows

$$\lambda_{2,1/2} \simeq 1.55524 > 1.46436\cdots = (1/1.647\, C_{2,1.2140})^{1/2}. \tag{2.43}$$

3. Numerical Experiments

In order to assess the quality of the estimates (1.31), (1.32), (1.36) and (1.37) we have calculated the numbers $\lambda_{N,\theta}$ for $N = 2, 3$ and $\theta = 0.1 + (i - 1)0.005$, $i = 1, 2, 3, \cdots, 180$, and for $N = 4, 5, 10$, and $\theta = 0.0125 + (i - 1)0.025$, $i = 1, 2, 3, \cdots, 40$. For $N = 2$ we had to exclude $\theta \geq 0.945$ due to numerical overflow. The method to find $\lambda_{N,\theta}$ consists of a shooting technique to find that value $v(0) = v_0$ such that $v(r)$ is a positive solution of (2.1) with $\lim_{r\to\infty} v(r) = 0$. Therefore, we transformed the interval $r \in (0, \infty)$ into $s = r/(1 + r) \in (0, 1)$. The transformed differential equation becomes, with $v(r) = u(s)$, $0 < s < 1$,

$$(1-s)^4 \frac{d^2}{ds^2} u + \left\{ \left(\frac{(N-1)}{s} - 2 \right) (1-s)^3 \right\} \frac{d}{ds} u - u|u|^{(N+2\theta)/(N-2\theta)-1} - u = 0,$$

$$u(0) = v_0, \qquad \frac{d}{ds} u(0) = 0. \tag{3.1}$$

We solved the transformed differential equation (3.1) by means of a numerical integration method (Runge-Kutta of the fourth order) with a self-adapting step-size routine such that a prescribed maximal relative error (ε_{rel}) in each component $(u(s), \frac{d}{ds}u(s))$ has been satisfied. We made the choice $\varepsilon_{rel} = 10^{-15}$. For every value of v_0 the numerical integrator will find some point $s = s(v_0) \in (0, 1)$ where either $u(s) < 0$, or $\frac{d}{ds}u(s) > 0$. At that point s the integration will be stopped. This integrator is coupled to a numerical zero-finding routine (see [4]), which can also be applied for finding a discontinuity. The function f for which such a discontinuity has to been found is specified by if $u(s(v_0)) < 0$,

$f(v_0) = -(1-s(v_0))$ else (that means thus $\frac{d}{ds}u(s(v_0)) > 0$) $f(v_0) = (1-s(v_0))$. The sought value v_0 has been found if this numerical routine has come up with two values v_0 and v_0^1 such that $|v_0 - v_0^1| < r_p|v_0| + a_p$, (with $r_p = a_p = 10^{-15}$ relative and absolute precisions, respectively) and $|f(v_0)| \leq |f(v_0^1)|$, while $sign(f(v_0) = -sign(f(v_0^1))$. During the integration processes the norms in (2.9) will be calculated. As a check upon this procedure the following expressions

$$\|\bar{v}_{N,\theta}\|_2^2/(1-\theta), \quad \|\nabla\bar{v}_{N,\theta}\|_2^2/\theta, \quad \|\bar{v}_{N,\theta}\|_r^r, \tag{3.2}$$

are compared. They should be all equal, see (2.9). In the Table 1 the value for $\lambda_{N,\theta}$ are given with one digit less than the number of equal digits in this comparison; between brackets the next digit is given.

The results of the calculations are shown in the Figures 1, 3, 5, 6, 7. For $N = 2, 3$ part of the θ-range has been enlarged to show better the approximations and the infimum of the functional, see Figures 2, 4. (All figures appear in Appendix A at the end of this paper.)

In Fig. 13 the value $v(0)$ of the minimizer $v(r)$ of the functional $\Lambda_{N,\theta}$ as function of θ for $N = 2, 3, 4, 5, 10$ has been shown. Note the logarithmic ordinate axis for $v(0)$.

N	θ	p	s	ρ	$\lambda_{N,\theta}$ numerical	$\lambda_{N,\theta}$ lower bnd.	Comment
2	$1/3$	3	$1/2$	1	1.379427(6)		numerical, this work
						1.28953	see (1.32), this work
						N.A.	see (1.31), this work
						1.37026	see (1.42), Nasibov
						1.35157	see (1.45), Nasibov
2	$1/2$	2	1	2	1.55524		numerical (2.12), based on Weinstein [29]
					1.555239(5)		numerical, this work
						1.46436	see (1.32), this work
						1.33134	see (1.31), this work
						1.51739	see (1.42), Nasibov
						1.51739	see (1.45), Nasibov
2	$2/3$	$3/2$	2	4	1.66287		numerical (2.13), based on Levine [13]
					1.663066(0)		numerical, this work
						1.63696	see (1.32), this work
						1.63696	see (1.31), this work
						1.55436	see (1.42), Nasibov
						1.61962	see (1.45), Nasibov
3	$3/4$	2	1	2	2.2258(9)		numerical, this work
						2.21005	see (1.32), this work
						2.21005	see (1.31), this work
						2.05668	see (1.42), Nasibov
						2.05668	see (1.45), Nasibov

Table 1: Comparison of some cases for $\lambda_{N,\theta}$; $p = N/(2\theta)$; $s = 2\theta/(N-2\theta)$ (notation Weinstein); $\rho = 4\theta/(N-2\theta)$ (notation Nasibov).

4. Discussion

In this article the infimum of the spectrum of the Schrödinger operator $\tau = -\Delta + q$ in $\mathbb{R}^N$ has been expressed in the infimum $\lambda_{N,\theta}$ of the functional $\Lambda_{N,\theta}$, and known estimates for $\lambda_{N,\theta}$ have been optimized and applied to supply estimates of the infimum of the spectrum. Moreover, numerical experiments have been done to calculate $\lambda_{N,\theta}$ as function of θ for $N = 2, 3, 4, 5$, and 10. These results have been used to compare the estimates found in this article with these found by Nasibov [20].

Except for $N = 2$, in general, the estimate of Nasibov is better for the lower half of the θ-interval, while the estimate in this article is better for the upper half. For $N = 2$ there is an interval (θ_-,θ_+) (with $\theta_- \in (0.615, 0.620)$, and $\theta_+ \in (0.745, 0.750)$) where the bound in this article is better, while the opposite is true outside that interval, see Fig. 8. For $0 < \theta \leq \theta_0$ (where $\theta_0 \in (0.55, 0.65)$ is depending on the value of N, $N = 3, 4, 5, 10$), the lower bound by Nasibov is better, but the bounds are of the same order of magnitude and very close to the actual value of $\lambda_{N,\theta}$; for $\theta_0 < \theta < 1$, the bound of Nasibov is worse, see Figs. 9, 10, 11, and 12.

The ratio of the estimate in this article with $\lambda_{N,\theta}$, for $\theta \to 1$, $N \geq 3$, approaches the value 1, since $\lambda_{N,1} = C_{N,2}$, $N \geq 3$ (see just after (1.16) and the Figs. 9, 10, 11, and 12).

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References

[1] R.A. ADAMS, *Sobolev Spaces*, Academic Press, New York 1975.

[2] T. AUBIN, Problèmes isopérimétriques et espaces de Sobolev, *J. Differential Geom.*, **11** (1976), 573–598.

[3] C. BENNEWITZ AND E.J.M. VELING, Optimal bounds for the spectrum of a one-dimensional Schrödinger operator, in *General Inequalities 6* (Edited by W. WALTER), International Series of Numerical Mathematics, vol. 103, Birkhäuser Verlag, Basel, 6th International Conference on General Inequalities, December 9-15, 1990, Oberwolfach 1992, pp. 257–268.

[4] J.C.P. BUS AND T.J. DEKKER, Two efficient algorithms with guaranteed convergence for finding a zero of a function, *ACM Trans. Math. Software*, **1**(4) (1975), 330–345.

[5] C.B. CLEMONS AND C.K.R.T. JONES, A geometric proof of the Kwong-McLeod uniqueness result, *SIAM J. Math. Anal.*, **24**(2) (1993), 436–443.

[6] M.S.P. EASTHAM AND H. KALF, *Schrödinger-type operators with continuous spectra*, Research Notes in Mathematics, vol. 65, Pitman, London 1982.

[7] D.E. EDMUNDS AND W.D. EVANS, *Spectral Theory and Differential Operators*, Oxford Mathematical Monographs, Oxford University Press, Oxford 1990.

[8] W.N. EVERITT, On the spectrum of a second order linear differential equation with a p-integrable coefficient, *Appl. Anal.*, **2** (1972), 143–160.

[9] J. GUNSON, Inequalities in Mathematical Physics, in *Inequalities, Fifty Years On from Hardy, Littlewood and Pólya* (Edited by W. NORRIE EVERITT), Lecture Notes in Pure and Applied Mathematics Series, no. 129, London Mathematical Society, Marcel Dekker, Inc., New York, Basel, Hong Kong, Proceedings of the International Conference, July 13-17, 1987, University of Birmingham, U.K. 1991, pp. 53–79.

[10] B.J. HARRIS, Lower bounds for the spectrum of a second order linear differential equation with a coefficient whose negative part is p-integrable, *Proc. Roy. Soc. Edinburgh Sect. A*, **97** (1984), 105–107.

[11] MAN KAM KWONG, Uniqueness of positive solutions of $\Delta u - u + u^p = 0$ in $\mathbf{R}^N$, *Arch. Ration. Mech. Anal.*, **105**(3) (1989), 243–266.

[12] MAN KAM KWONG AND LIQUN ZHANG, Uniqueness of the positive solution of $\Delta u + f(u) = 0$ in an annulus, *Differential Integral Equations*, **4**(3) (1991), 583–599.

[13] H.A. LEVINE, An estimate for the best constant in a Sobolev inequality involving three integral norms, *Ann. Mat. Pura Appl. (4)*, **124** (1980), 181–197.

[14] E.H. LIEB, Sharp constants in the Hardy-Littlewood-Sobolev and related inequalities, *Ann. of Math.*, **118**(2) (1983), 349–374.

[15] E.H. LIEB AND W.E. THIRRING, Inequalities for the moments of the eigenvalues of the Schrödinger Hamiltonian and their relation to Sobolev

inequalities, in *Studies in Mathematical Physics, Essays in Honor of Valentine Bargmann* (Edited by E. H. LIEB, B. SIMON AND A. S. WIGHTMAN), Princeton University Press, Princeton 1976, pp. 269–303.

[16] E.H. LIEB, Bounds on Schrödinger Operators and Generalized Sobolev-Type Inequalities with Applications in Mathematics and Physics, in *Inequalities, Fifty Years On from Hardy, Littlewood and Pólya* (Edited by W. NORRIE EVERITT), Lecture Notes in Pure and Applied Mathematics Series, no. 129, London Mathematical Society, Marcel Dekker, Inc., New York, Basel, Hong Kong, Proceedings of the International Conference, July 13-17, 1987, University of Birmingham, U.K. 1991, pp. 123–133.

[17] K. McLEOD AND J. SERRIN, Uniqueness of solutions of semilinear Poisson equations, *Proc. Nat. Acad. Sci. USA*, **78**(11) (1981), 6592–6595.

[18] K. McLEOD AND J. SERRIN, Uniqueness of positive radial solutions of $\Delta u + f(u) = 0$ in $\mathbf{R}^N$, *Arch. Ration. Mech. Anal.*, **99** (1987), 115–145.

[19] B. v. Sz. NAGY, Űber Integralungleichungen zwischer einer Funktion und ihrer Ableitung, *Acta Sci. Math. (Szeged)*, **10** (1941), 64–74.

[20] Sh. M. NASIBOV, On optimal constants in some Sobolev inequalities and their application to a nonlinear Schrödinger equation, *Soviet. Math. Dokl.*, **40**(1) (1990), 110–115, translation of *Dokl. Akad. Nauk SSSR* **307**(3) (1989), 538-542.

[21] M. REED AND B. SIMON, *Methods of Modern Mathematical Physics II: Fourier Analysis, Self-Adjointness*, Academic Press, New York 1975.

[22] M. REED AND B. SIMON, *Methods of Modern Mathematical Physics I: Functional Analysis*, Academic Press, New York 1980, Revised and enlarged edn.

[23] G. ROSEN, Necessary conditions on potential functions for nonrelativistic bound states, *Phys. Rev. Lett.*, **49** (1982), 1885–1887.

[24] W.A. STRAUSS, Existence of solitary waves in higher dimensions, *Comm. Math. Phys.*, **55** (1977), 149–162.

[25] G. TALENTI, Best constant in Sobolev inequality, *Ann. Mat. Pura Appl.*, **110**(4) (1976), 353–372.

[26] W. THIRRING, *A Course in Mathematical Physics III. Quantum Mechanics of Atoms and Molecules*, Springer, New York 1981.

[27] E.J.M. VELING, Optimal lower bounds for the spectrum of a second order linear differential equation with a p-integrable coefficient, *Proc. Roy. Soc. Edinburgh Sect. A*, **92** (1982), 95–101.

[28] E.J.M. VELING, *Transport by Diffusion*, Ph.D. thesis, University of Leiden, Leiden, The Netherlands (1983).

[29] M.I. WEINSTEIN, Nonlinear Schrödinger equations and sharp interpolation estimates, *Comm. Math. Phys.*, **87** (1983), 567–576.

A. Figures

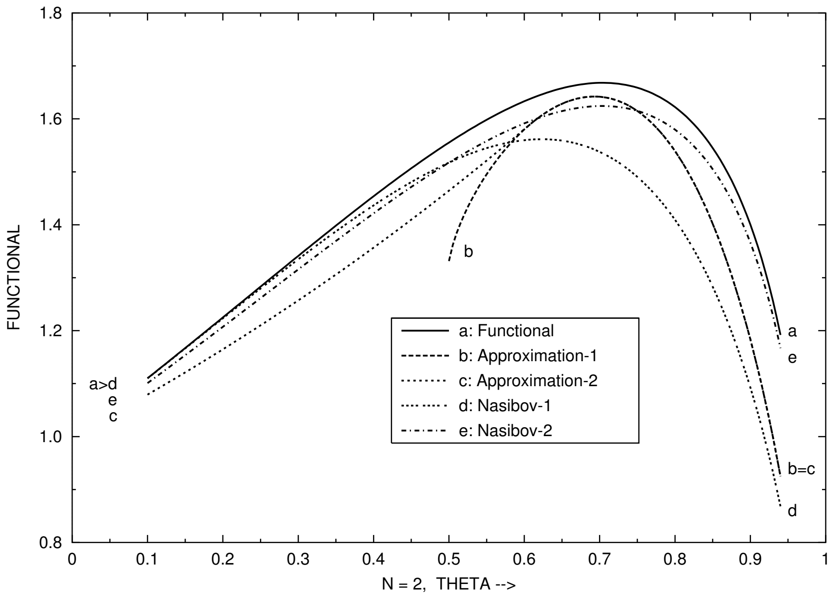

Figure 1: $N = 2$: $\lambda_{2,\theta}$ with four approximations; Approximation-1 corresponds with Theorem 1.2-(ii), Approximation-2 with Theorem 1.2-(iii), Nasibov-1 with (1.43), Nasibov-2 with (1.46).

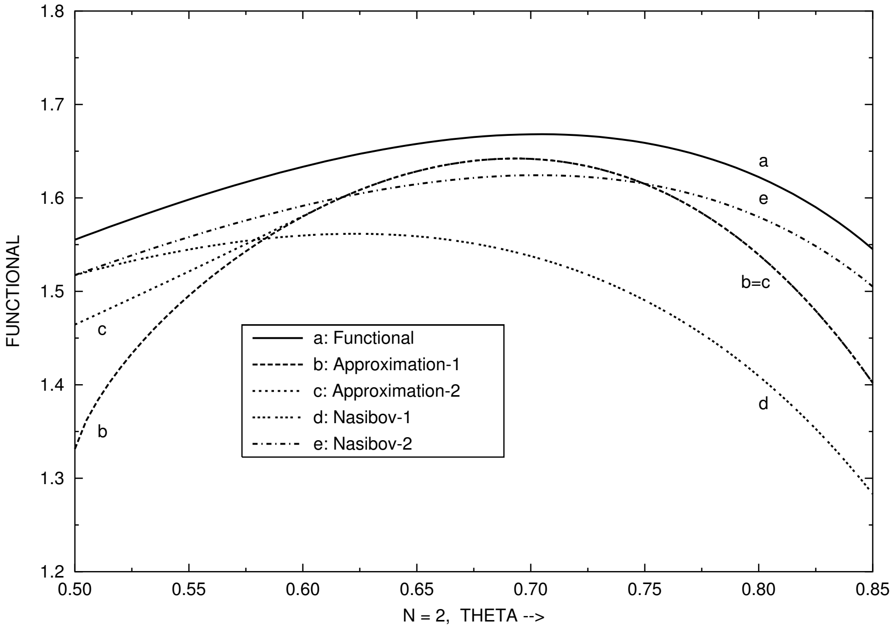

Figure 2: $N = 2$: $\lambda_{2,\theta}$ with four approximations; Approximation-1 corresponds with Theorem 1.2-(ii), Approximation-2 with Theorem 1.2-(iii), Nasibov-1 with (1.43), Nasibov-2 with (1.46).

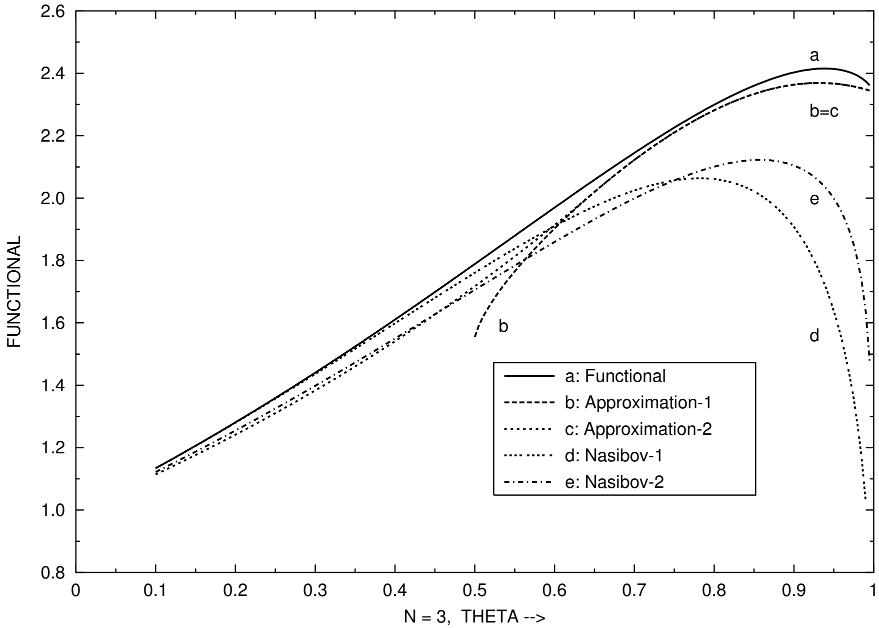

Figure 3: $N = 3$: $\lambda_{3,\theta}$ with four approximations; Approximation-1 corresponds with Theorem 1.2-(ii), Approximation-2 with Theorem 1.2-(iii), Nasibov-1 with (1.43), Nasibov-2 with (1.46).

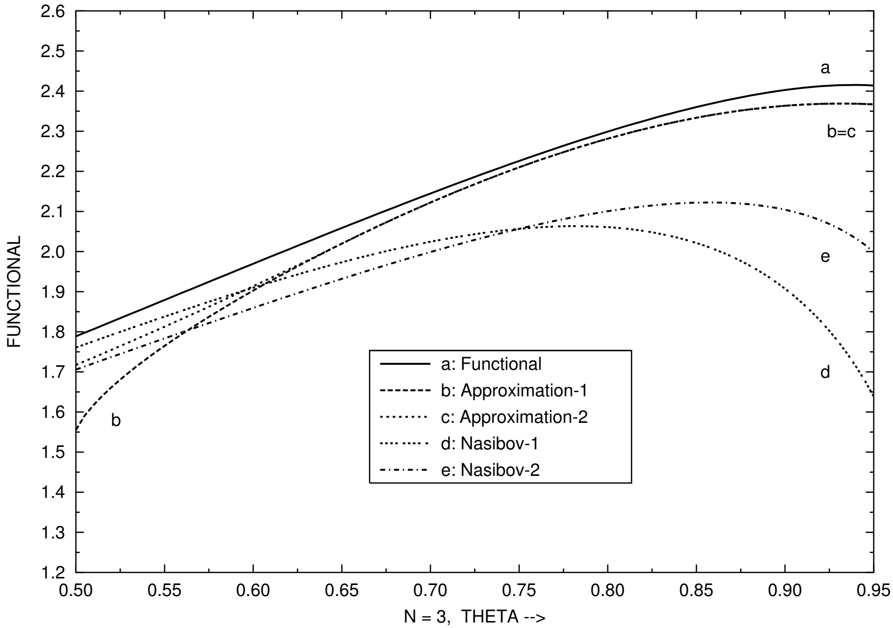

Figure 4: $N = 3$: $\lambda_{3,\theta}$ with four approximations; Approximation-1 corresponds with Theorem 1.2-(ii), Approximation-2 with Theorem 1.2-(iii), Nasibov-1 with (1.43), Nasibov-2 with (1.46).

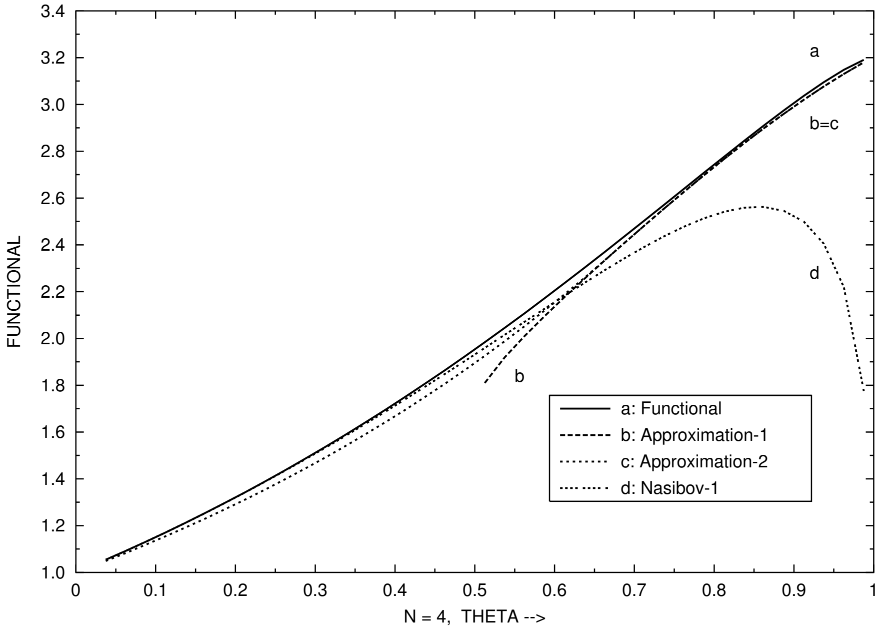

Figure 5: $N = 4$: $\lambda_{4,\theta}$ with three approximations; Approximation-1 corresponds with Theorem 1.2-(ii), Approximation-2 with Theorem 1.2-(iii), Nasibov-1 with (1.43).

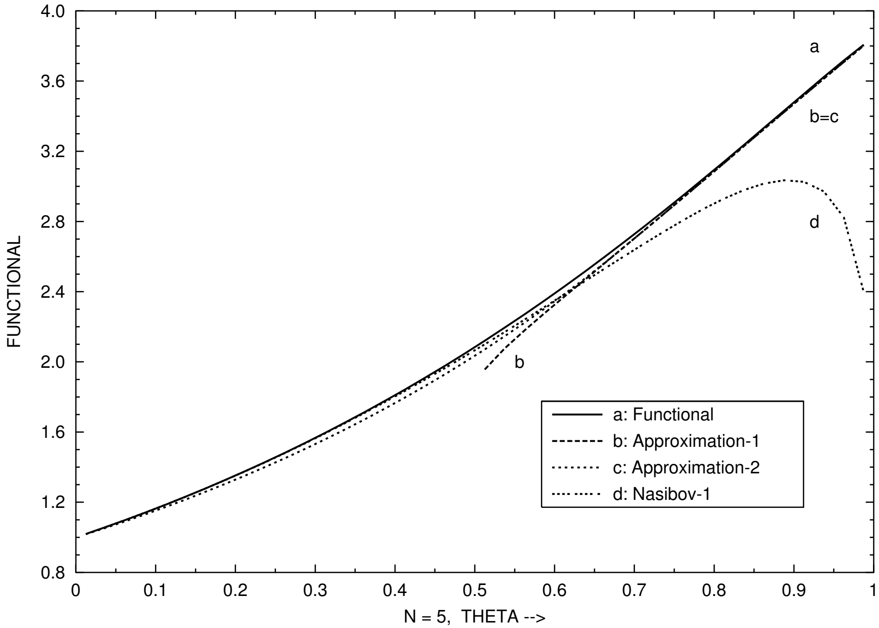

Figure 6: $N = 5$: $\lambda_{5,\theta}$ with three approximations; Approximation-1 corresponds with Theorem 1.2-(ii), Approximation-2 with Theorem 1.2-(iii), Nasibov-1 with (1.43).

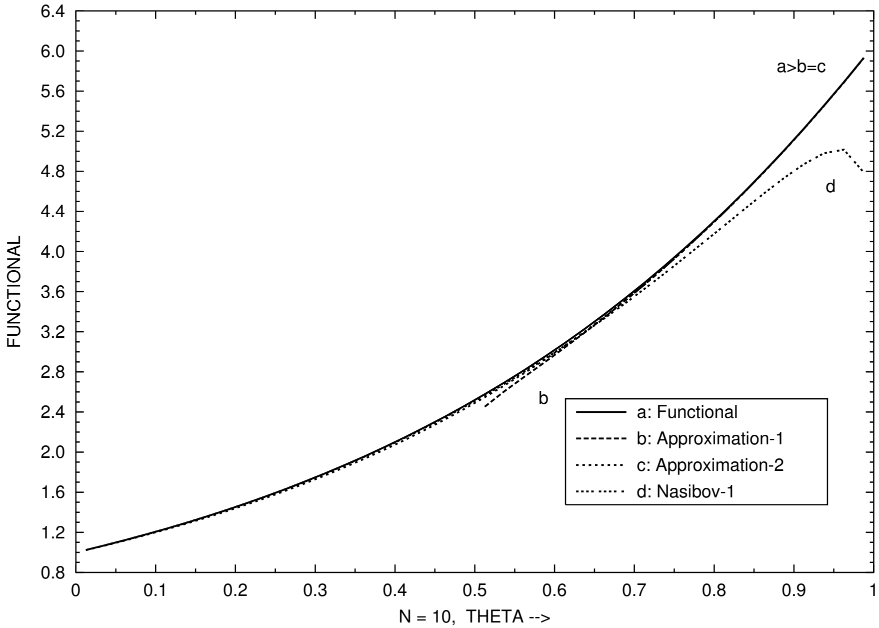

Figure 7: $N = 10$: $\lambda_{10,\theta}$ with three approximations; Approximation-1 corresponds with Theorem 1.2-(ii), Approximation-2 with Theorem 1.2-(iii), Nasibov-1 with (1.43).

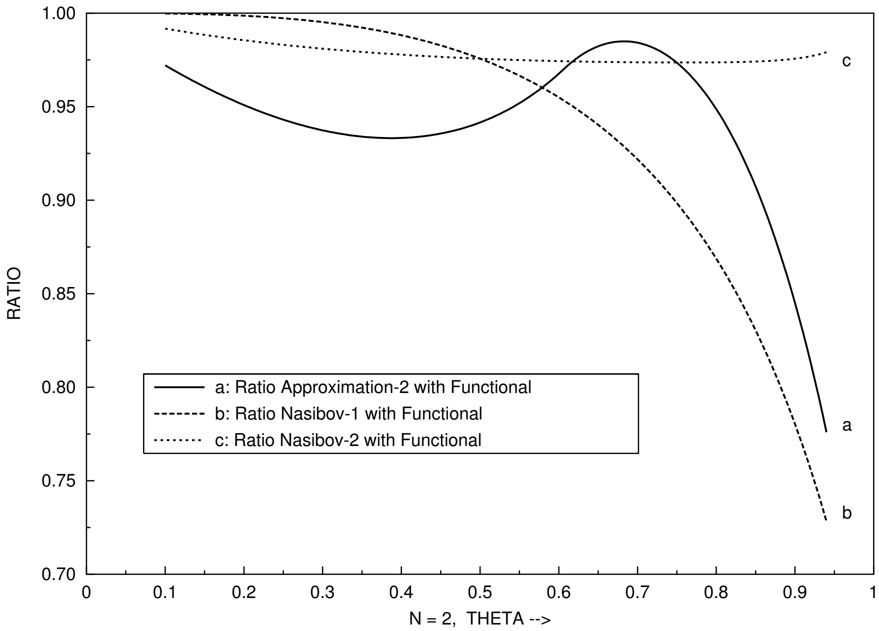

Figure 8: $N = 2$: Ratio of three approximations with $\lambda_{2,\theta}$: Approximation-2 (Theorem 1.2-(iii)), Nasibov-1 (1.43), and Nasibov-2 (1.46).

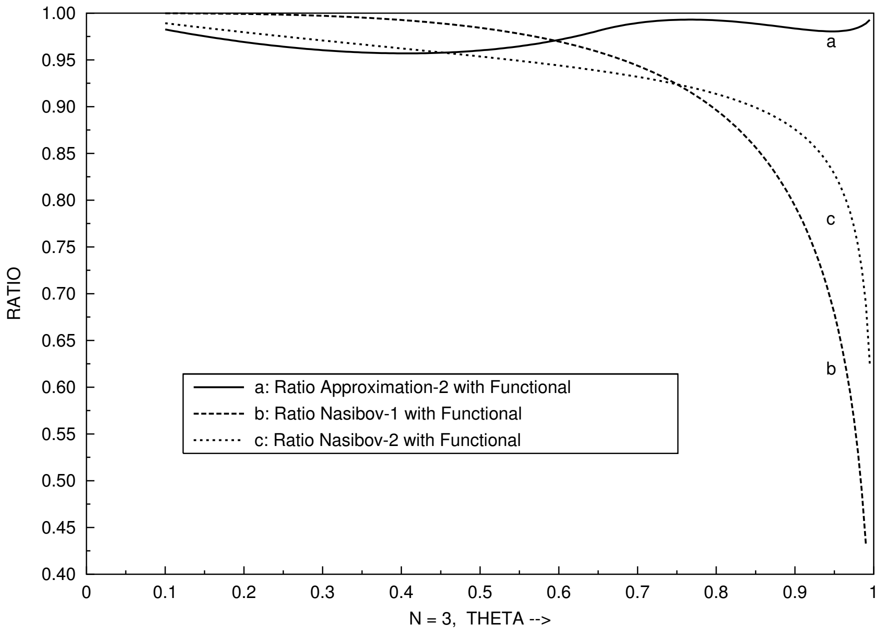

Figure 9: $N = 3$: Ratio of three approximations with $\lambda_{3,\theta}$: Approximation-2 (Theorem 1.2-(iii)), Nasibov-1 (1.43), and Nasibov-2 (1.46).

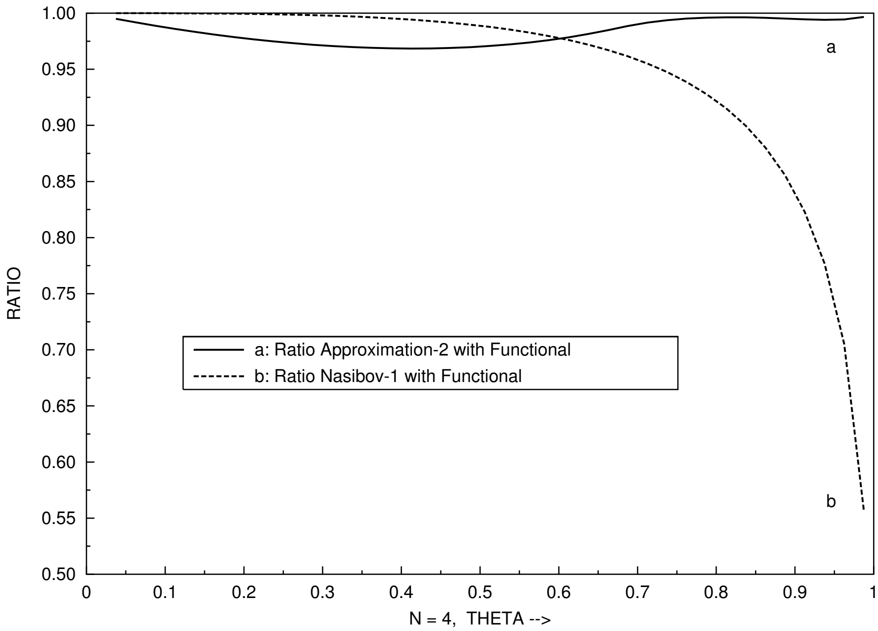

Figure 10: $N = 4$: Ratio of two approximations with $\lambda_{4,\theta}$: Approximation-2 (Theorem 1.2-(iii)) and Nasibov-1 (1.43).

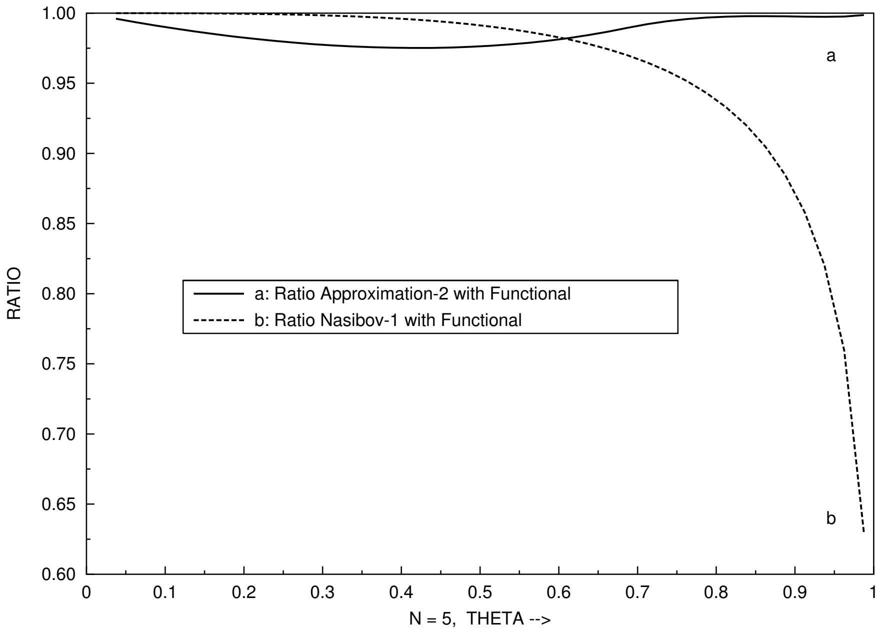

Figure 11: $N = 5$: Ratio of two approximations with $\lambda_{5,\theta}$: Approximation-2 (Theorem 1.2-(iii)) and Nasibov-1 (1.43).

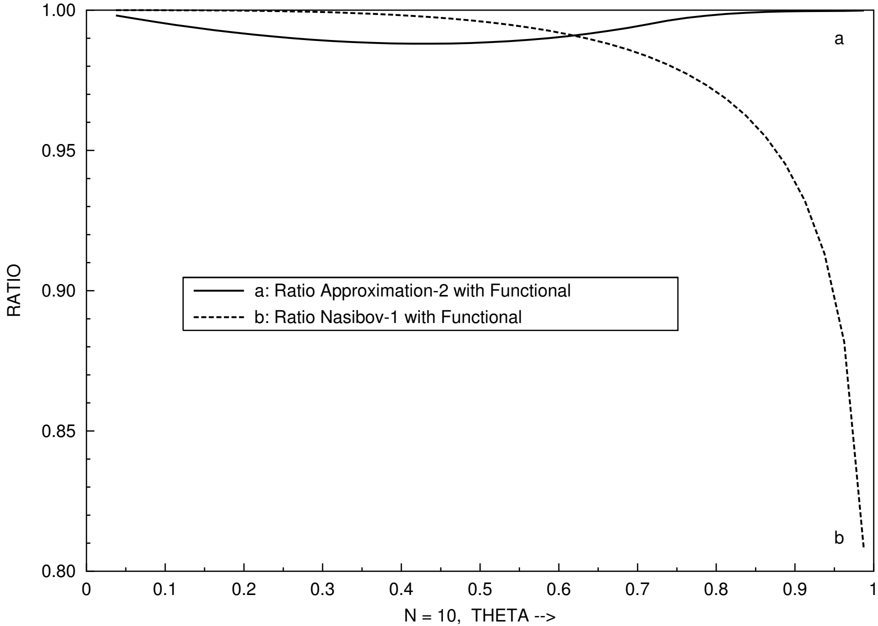

Figure 12: $N = 10$: Ratio of two approximations with $\lambda_{10,\theta}$: Approximation-2 (Theorem 1.2-(iii)) and Nasibov-1 (1.43).

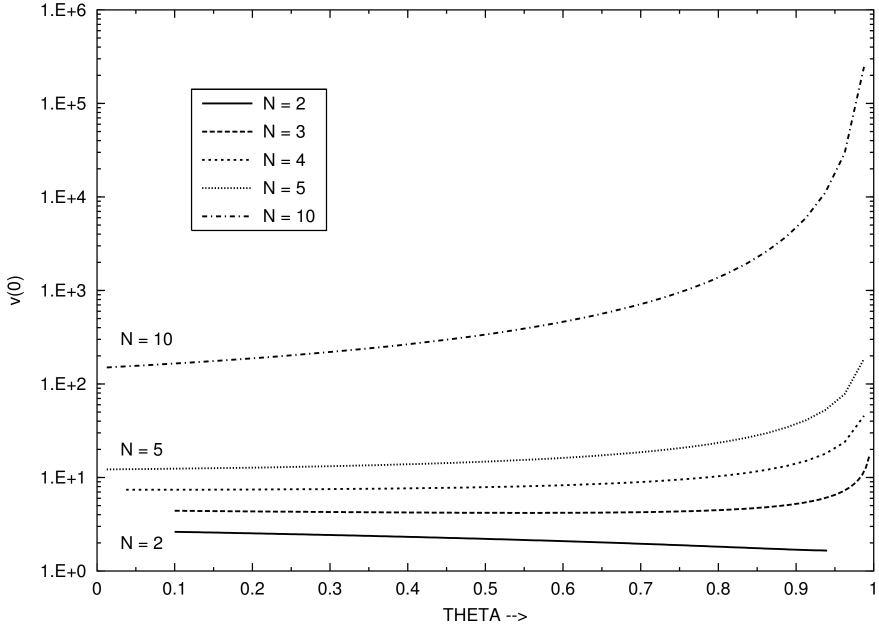

Figure 13: The value $v(0)$ of the minimizer $v(r)$ of the functional $\Lambda_{N,\theta}$ as function of θ for $N = 2, 3, 4, 5, 10$.