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Asymptotics for the Approximation of Wave Functions by Exponential Sums

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When studying the approximation of the wave functions of the H-atom by sums of Gaussians, Klopper and Kutzelnigg [KK] and Kutzelnigg [Ku] found an asymptotic of $\exp[-\gamma\sqrt{n}]$. The results were obtained from numerical results and justified by some asymptotic expansions in quadrature formulas. We will verify the asymptotic behaviour by a very different method. We transform the given problem into an approximation problem of completely monotone functions by exponential sums. The approximation problem on an infinite interval is treated by using results from rational approximation.

1. Introduction

When studying wave functions of the H-atom, Kutzelnigg [Ku] started from the observation that the function $e^{-\alpha r}$ and $1/r$ can be expressed as Gaussian integral transforms:

$$e^{-\alpha r} = \frac{\alpha}{2\sqrt{\pi}} \int_0^\infty s^{-3/2} \exp[-\frac{\alpha^2}{s} - sr^2] ds, \tag{1.1}$$

$$\frac{1}{r} = \frac{1}{\sqrt{\pi}} \int_0^\infty s^{-1/2} e^{-sr^2} ds. \tag{1.2}$$

Therefore by using quadrature formulas, the functions were approximated by Gaussian sums

$$u_n(r) = \sum_{k=1}^n \alpha_k e^{\beta_k r^2}.$$

The error of approximation was given by Kutzelnigg [Ku] in terms of the error of the expectation value of an energy. In order to measure the degree of approximation in a rigorous mathematical way, we will consider a norm of the error function $\|f - u_n\|$. Since the approximation is to be performed such that the mentioned expectation value for the H-atom can be evaluated with good accuracy, the weighted L_1-norm

$$\|g\| := \int_0^\infty r^2 |g(r)| e^{-r} dr \tag{1.3}$$

is the natural choice. To be more precise, there was an additional parameter in the exponent on the right hand side of (1.3), but it is not difficult to see that the parameter can be eliminated by a simple scale transformation, see (4.3) below.

Numerical calculations by Kutzelnigg showed an asymptotic law

$$\approx e^{-\pi\sqrt{n/3}} \tag{1.4}$$

for the approximation of $1/r$. Seeing his result we expect an error with a behaviour of the form

$$\|f - u_n\| = O(e^{-\gamma\sqrt{n}}). \tag{1.5}$$

We have attacked the approximation problem in a different way and have used an idea which can be found already in the approximation by exponential sums, see [Braess 1986, pp. 177–178]. By the simple transformation of the variable $x = r^2$ we find that the given functions (1.1) and (1.2) are completely monotone and that they are to be approximated by exponential sums. The degree of approximation can now be estimated by the maximum principle and well-known results from rational approximation. In contrast to the earlier results, we have to deal with infinite intervals. For this reason, the estimates are based on different results on rational approximation. Moreover, we perform a cut-off in the direct variable as well as in the spectrum. We obtain an asymptotic law with

$$\gamma = 2\pi\sqrt{1/3}. \tag{1.6}$$

The exponent γ is twice the value of the result (1.4) from [Ku]. We note that an improvement with a doubling of an exponent is often found in nonlinear approximation problems when some extra parameters are considered free.

In order to keep the formalism at a low level, we will restrict ourselves to the approximation problems with the weighted L_1-norm (1.3). The reader can easily see how the technique may be generalized.

Our method provides only upper estimates. Therefore we report on some improved numerical results for an older example which shows that the method yields often sharp estimates.

2. An Error Estimate for Completely Monotone Functions

When we heard of the $e^{-\text{const}\sqrt{n}}$ behaviour, we were immediately reminded of a problem in uniform rational approximation which has this behaviour. Due to Stahl [1992] one has

$$\lim_{n\to\infty} e^{\pi\sqrt{n}} E_{n,n}(|x|, [-1,1]) = 8. \tag{2.1}$$

Here $E_{m,n}$ is the degree of uniform approximation from $R_{m,n}$, i.e., the approximation by rational functions whose numerators are polynomials in Π_m and whose denominators are in Π_n. Moreover, from Varga, Ruttan, and Carpenter [VRC] one knows that the limes is reached from below.

When the asymptotics for $E_{n,n}(|x|, [-1,1])$ is determined, usually estimates for the auxiliary function $xp(x)/p(-x)$ are established where p is a suitable polynomial in Π_n, see e.g. Newman [1964]. In order to derive L_1-estimates, we need a similar auxiliary function.

Lemma 1. *Let $n \geq 1$ and $\alpha > 0$. Then there exists a polynomial $p \in \Pi_n$ with n zeros in $[0, 1]$ such that*

$$\left| x^\alpha \frac{p(x)}{p(-x)} \right| \leq c_0(\alpha) \cdot e^{-\pi\sqrt{\alpha n}} \quad \text{for } 0 \leq x \leq 1. \tag{2.2}$$

The lemma is essentially Lemma 4 of Vjačeslavov [1977]. We will first use it for $\alpha = 3/2$. By standard arguments we conclude from (2.1) that we have $c_0(\alpha) \leq \sqrt{2} \cdot 8^{3/2}$, i.e.,

$$c_0 \leq 32 \quad \text{for } \alpha = \frac{3}{2} \tag{2.3}$$

at least if (2.2) is used for sufficiently large n. Moreover, the number 32 is not far from the best bound.

A function

$$f(z) = \int_0^\infty e^{-sz} d\mu(s)$$

is called a *completely monotone* function, if $d\mu$ is a nonnegative measure. If $\int d\mu(s) < \infty$, then f is bounded in the right half plane and

$$|f(z)| \leq f(0) \quad \text{for } \operatorname{Re} z \geq 0. \tag{2.4}$$

A function of the form

$$\sum_{k=1}^n \alpha_k e^{\beta_k x}$$

is called an exponential sum of order n.

The following result is an adaptation of a Lemma in [B, p. 177].

Lemma 2. *Assume that f is completely monotone and bounded for $\operatorname{Re} z > 0$. Moreover let $b > 0$ and $c_0 = c_0(3/2)$ be as above. Then there is an exponential sum u_n of order n such that*

$$x^{3/2}|f(x) - u_n(x)| \leq 2b^{3/2} f(0)\, c_0 e^{-\pi\sqrt{3n}} \quad \text{for } 0 \leq x \leq b. \tag{2.5}$$

Proof. From Lemma 1 we know that there is a polynomial q with $2n$ zeros in $(0, 1)$ such that

$$\left| x^{3/2} \frac{q(x)}{q(-x)} \right| \leq c_0 e^{-\pi\sqrt{3n}} \quad \text{for } x \in [0, 1].$$

By setting $p(x) = q(x/b)$ we obtain

$$\left| x^{3/2} \frac{p(x)}{p(-x)} \right| \leq b^{3/2} c_0 e^{-\pi\sqrt{3n}} \quad \text{for } x \in [0, b]. \tag{2.6}$$

Since f is completely monotone, there exists an exponential sum u_n of order n which interpolates f at the $2n$ zeros

$$x_1 \leq \ldots \leq x_{2n}$$

counting multiplicities, see [B, p. 176]. Since $f - u_n$ cannot have more than $2n$ zeros, it follows that $u_n(x) \le f(x)$ for $x \le x_1$ and for $x \ge x_{2n}$. From this we know that $u_n(0) \le f(0)$ and

$$|f(z) - u_n(z)| \le |f(z)| + |u_n(z)| \le f(0) + u_n(0) \le 2f(0) \quad \text{for } \mathrm{Re}\, z \ge 0. \tag{2.7}$$

The function

$$g(z) := \frac{p(-x)}{p(x)}[f(z) - u_n(z)]$$

is analytic in the right half plane. Moreover we know that

$$\begin{aligned} \left|\frac{q(-z)}{q(z)}\right| &= 1 \quad \text{for } \ \mathrm{Re}\ z = 0, \\ \frac{q(-z)}{q(z)} &\to 1 \quad \text{for } |z| \to \infty. \end{aligned}$$

Hence, by the maximum principle

$$|g(z)| \le 2f(0) \quad \text{for } \mathrm{Re}\, z \ge 0. \tag{2.8}$$

Finally, we conclude from (2.6) and (2.8) that

$$x^{3/2}|f(z) - u_n(z)| = |x^{3/2}\frac{q(x)}{q(-x)}| \cdot |g(z)| \le b^{3/2} c_0 e^{-\pi\sqrt{3n}} \quad \text{for } x \in [0, b],$$

and the proof is complete. □

Remark 3. If we require the estimate (2.5) only for $a \le x \le b$, with some $a > 0$, then we may assume that all the zeros of $f - u_n$ are contained in $[a, b]$.

To understand this, we consider (2.2) once more. Assume that the polynomial p has a zero $x_1 \in (0, a)$. Choose $\tilde{x}_1 \in (a, \min[1, 2a - x_1])$. Obviously,

$$\left|\frac{x - \tilde{x}_1}{x + \tilde{x}_1}\right| \le \left|\frac{x - x_1}{x + x_1}\right| \quad \text{for } a \le x \le b.$$

Hence, we may redefine p and replace x_1 by $\tilde{x}_1$ without a change of the bound.

3. Approximation of $r^{-1/2}$

We will consider the approximation with respect to the weighted L_1-norm

$$\|g\| := \int_0^\infty \sqrt{x}\, |g(x)| e^{-\sqrt{x}} dx \tag{3.1}$$

$$= 2\int_0^\infty r^2 |g(r^2)| e^{-r} dr. \tag{3.2}$$

It seems to be natural to split the infinite interval into 3 parts: $[0,\infty) = [0,m] \cup [m,M] \cup [M,\infty]$. In the domain $[m,M]$ we will use a weigthed sup-norm of the interpolation error. On the other hand, in $[0,m] \cup [M,\infty]$ we will have $0 < u_n < f$, and the contribution of these parts to $\|f - u_n\|$ may be estimated by the contribution of $|f|$ only.

First we consider the function

$$f(x) := x^{-1/2} = \frac{1}{\sqrt{\pi}} \int_0^\infty s^{-1/2} e^{-sx} ds \tag{3.3}$$

Here we have

$$\int_0^m \sqrt{x} \frac{1}{\sqrt{x}} e^{-\sqrt{x}} dx \leq m, \tag{3.4}$$

$$\int_M^\infty \sqrt{x} \frac{1}{\sqrt{x}} e^{-\sqrt{x}} dx = 2 \int_{\sqrt{M}}^\infty r e^{-r} dr = (\sqrt{M} + 1)\, e^{-\sqrt{M}}. \tag{3.5}$$

Since our aim is an estimate of the form

$$\|f - u_n\| \leq c n^{3/2} e^{-\gamma\sqrt{n}} \tag{3.6}$$

with $\gamma = \pi\sqrt{4/3}$, we will set

$$m = m(n) := \frac{4}{3}\pi^2 n e^{-\pi\sqrt{(4/3)n}}, \qquad M = M(n) := \frac{4}{3}\pi^2 n. \tag{3.7}$$

The function f is not bounded in the right half-plane. Therefore, referring to the representation (3.3) we will also perform a cut-off in the s-variable and consider for $T > 0$

$$f_T(x) := \frac{1}{\sqrt{\pi}} \int_0^T s^{-1/2} e^{-sx} ds. \tag{3.8}$$

We have

$$f(x) - f_T(x) = \frac{1}{\sqrt{\pi}} \int_T^\infty s^{-1/2} e^{-sx} ds \leq \frac{1}{\sqrt{\pi T}} \int_T^\infty e^{-sx} ds = \frac{1}{x\sqrt{\pi T}} e^{-Tx}.$$

By using (3.2) we evaluate a bound of the norm

$$\begin{aligned} \|f - f_T\| &\leq \frac{2}{\sqrt{\pi T}} \int_0^\infty e^{-Tr^2} e^{-r} dr \\ &\leq \frac{2}{\sqrt{\pi T}} \int_0^\infty e^{-Tr^2} dr = T^{-1}. \end{aligned} \tag{3.9}$$

Note that

$$f_T(0) = \frac{1}{\sqrt{\pi}} \int_0^T s^{-1/2} ds = \frac{2}{\sqrt{\pi}} T^{1/2}. \tag{3.10}$$

With respect to our aim we will set

$$T = T(n) := (64\pi^3 n)^{-1} e^{+\gamma\sqrt{n}}. \tag{3.11}$$

Theorem 4. *For any $n \geq 1$ there exists an exponential sum u_n of order n which satisfies*

$$\|x^{-1/2} - u_n\| \leq c n^{3/2} e^{-\gamma\sqrt{n}} \tag{3.12}$$

with $\gamma = 2\pi\sqrt{1/3}$ and c a number independent of n.

Proof. We apply Lemma 2 to f_T with $T = (64\pi^3 n)^{-1} e^{+\gamma\sqrt{n}}$ and $b = M(n) = 3\pi^2 n$. We obtain for $0 \leq x \leq b$

$$\begin{aligned} x^{3/2}|f_T(x) - u_n(x)| &\leq 2(3\pi^2 n)^{3/2} \frac{2}{\sqrt{\pi}} (64\pi^3 n)^{-1/2} e^{\gamma/2\sqrt{n}} (32 e^{-\pi\sqrt{3n}}) \\ &= 48\sqrt{3} n e^{(\gamma/2 - \pi\sqrt{3})\sqrt{n}}. \end{aligned} \tag{3.13}$$

Denote the right hand side of (3.13) by ϵ. We integrate the expression with the boundary points given in (3.7)

$$\begin{aligned} &\int_m^M \sqrt{x}\,|f_T(x) - u_n(x)| e^{-\sqrt{x}}\, dx \\ &\leq \int_m^M \frac{1}{x} \epsilon dx = \epsilon[\log M - \log m] = \epsilon\pi\sqrt{(4/3)n} = 96\pi^2 n^{3/2} e^{(\gamma/2 - \pi\sqrt{3})\sqrt{n}}. \end{aligned} \tag{3.14}$$

From Remark 3 we know that (3.14) holds for an exponential sum u_n which interpolates only at points in the interval $[m, M]$. Hence,

$$0 \leq u_n(x) \leq f_T(x) \leq f(x) \quad \text{for } x \in [0, m] \cup [M, \infty).$$

Therefore, the remaining parts of the integral for the calculation of $\|f_T - u_n\|$ can be estimated by (3.4) and (3.5) and we have

$$\|f_T - u_n\| \leq 100\pi^2 n^{3/2} e^{(\gamma/2 - \pi\sqrt{3})\sqrt{n}}.$$

Now we set $\gamma = \pi\sqrt{4/3} = \pi\sqrt{3} - \gamma/2$ and recall $\|f - f_T\| \leq T^{-1} = 64\pi^3 n e^{-\gamma\sqrt{n}}$. Summing up, we have for $n \geq 10$:

$$\|f - u_n\| \leq 164\pi^2 n^{3/2} e^{-\gamma\sqrt{n}}, \tag{3.15}$$

and the proof of (3.12) is complete. $\square$

4. Extensions and Other Methods

If the error is measured by the more general norm

$$\|g\|_\alpha := \int_0^\infty \sqrt{x}|g(x)|e^{-\sqrt{\alpha x}}dx, \tag{4.1}$$

with some $\alpha > 0$, then an appropriate exponential sum is obtained from the previous one by a simple transformation: Let u_n be the exponential sum of order n constructed in the previous section. Then

$$v_n(x) := \alpha^{1/2} \cdot u_n(\alpha x) \tag{4.2}$$

is also an exponential sum. We substitute $z = \alpha x$ when we determine the $\|\cdot\|_\alpha$ -norm of the error:

$$\begin{aligned}\Big\|\frac{1}{\sqrt{x}} - v_n\Big\|_\alpha &= \int_0^\infty \sqrt{x}\Big|\frac{1}{\sqrt{x}} - v_n(x)\Big|e^{-\sqrt{\alpha x}}dx \\ &= \int_0^\infty \sqrt{\alpha^{-1}z}\Big|\frac{1}{\sqrt{\alpha^{-1}z}} - \alpha^{1/2}u_n(z)\Big|e^{-\sqrt{z}}\frac{dz}{\sqrt{\alpha}} \\ &= \alpha^{-\frac{1}{2}}\Big\|\frac{1}{\sqrt{x}} - u_n\Big\|. \end{aligned} \tag{4.3}$$

The factor which results from the transformation, is independent of n.

On the other hand, there is a slower convergence to zero, if the error is considered for the L_2-norm. We obtain an approximant

$$\Big\|\frac{1}{\sqrt{x}} - u_n\Big\|_{L_2} := \Big[\int_0^\infty \sqrt{x}\Big|\frac{1}{\sqrt{x}} - u_n(x)\Big|^2 e^{-\sqrt{x}}dx\Big]^{1/2} \approx e^{-\pi\sqrt{n/6}}. \tag{4.4}$$

The smaller exponent is obtained, since Lemma 1 has to be used for $\alpha = \frac{3}{4}$ and the cut-off leads to $\|f - f_T\|_{L_2} \approx T^{-1/4}$. Here we choose $T \approx e^{4\pi\sqrt{n/6}}$ and $M \approx \pi^2 n/6$.

The method which we have used for getting bounds, provides also information how a good approximation can be obtained. We make use of the fact that the bounds in the rational approximation are obtained in a constructive way. We may choose $2n$ points which are equidistant after the transformation

$$x \longmapsto u = (\log\frac{x}{x_{\min}})^2, \qquad x \in [x_{\min}, x_{\max}],$$

with $x_{\min} = m(n)$, $x_{\max} = M(n)$, and compute the interpolating exponential sum. Kutzelnigg [Ku] on the other hand considered a transformation of the s-variable in the integral (3.3)

$$s \longmapsto t = \log\frac{s}{s_{\min}} \qquad s \in [s_{\min}, s_{\max}]$$

and replaced the integral by a finite sum, which refers to equally spaced points in the t-variable.

It is possibly too early for a conjecture which is the right exponent. In view of the results on a similar problem in Section 6, it is possible that (1.6) is the optimal result. On the other hand, it becomes also clear that we cannot expect to obtain the right polynomial term by our method. Thus, for convenience, we have not tried to improve the $n^{3/2}$-term. The constant in front of (3.15) is only given for curiosity and is not mentioned in Theorem 4.

5. Note on the Approximation of $e^{-\sqrt{x}}$

The analysis of the approximation process for the bounded function

$$f(x) := e^{-\sqrt{x}} = \frac{1}{2\pi}\int_0^\infty s^{-3/2}\exp\left(-\frac{1}{s}\right)e^{-sx}ds \tag{5.1}$$

is simpler for the following reason. Since $f(0) = 1 < \infty$, we do not need a cut-off in the s-variable and we do not get a deterioriation from $f(0)$. Also the contribution of small x to the norm has a nicer behaviour

$$\int_0^m \sqrt{x}f(x)e^{-\sqrt{x}}dx \le \int_0^m \sqrt{x}dx = \frac{2}{3}m^{3/2}. \tag{5.2}$$

Therefore we may choose $m \approx e^{-(2/3)\gamma\sqrt{n}}$ if we aim at a degree of approximation of $e^{-\gamma\sqrt{n}}$. Finally we obtain here

$$\|e^{-\sqrt{x}} - u_n\| \le cn^{3/2}e^{-\pi\sqrt{3n}}. \tag{5.3}$$

6. A Similar Problem with Sharp Bounds

Since we have established only upper bounds for the degree of approximation, we would like to present an argument that the bounds may not be too far the exact values.

For this reason we will report on results for the uniform approximation of the function $f(x) := 1/x$ by exponential sums on the interval $[1, 2]$. The estimates of Braess and Saff (see [B, pp. 177–179]) have been obtained by arguments which are analogous to those in Sections 2 and 3. Specifically, it was shown that the error E_n decreases according to the law

$$\lim_{n\to\infty}(E_n)^{1/n} \le \frac{1}{\omega^2}, \tag{6.1}$$

where the parameter ω for the interval $[1, 2]$ is given by

$$\omega^2 = \exp\frac{2\pi\mathsf{K}(\frac{1}{2})}{\mathsf{K}'(\frac{1}{2})} = 135.85281. \tag{6.2}$$

Here K and K' refer to elliptic integrals of second kind.

Some numerical results by Dünschede [1989] are presented in Table 1. It is surprising that the modified quotients

$$\frac{2n}{2n+1}\frac{E_{n-1}}{E_n}$$

are very close to the number given in (6.2). So there is the conjecture that equality holds in (6.1). By the way, from these numbers we expect that

$$E_n \approx c \cdot n^{1/2}\omega^{-2n}. \tag{6.3}$$

On the other hand, the cut off technique used in Section yields a bound with a factor n instead of $\sqrt{n}$. When we use the interpolant for $f_T(x) := \int_0^{2n\log\omega} e^{-sx}ds$, then we obtain the rigorous but weaker estimate

$$E_n \leq c \cdot n\,\omega^{-2n}. \tag{6.4}$$

Table 1. Uniform approximation of $1/x$ on $[1,2]$.

n	E_n	$\frac{E_{n-1}}{E_n}$	$\frac{2n}{2n-1}\frac{E_{n-1}}{E_n}$
1	$2.12794 \cdot 10^{-2}$		
2	$2.07958 \cdot 10^{-4}$	102.33	136.43
3	$1.83414 \cdot 10^{-6}$	113.38	136.06
4	$1.54170 \cdot 10^{-8}$	118.97	135.96
5	$1.26034 \cdot 10^{-10}$	122.32	135.92
6	$1.01179 \cdot 10^{-12}$	124.57	135.89
7	$0.802 \cdot 10^{-14}$	126.2	

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