A spectral method for Schrödinger equations with smooth confinement potentials

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Abstract We study the expansion of the eigenfunctions of Schrödinger operators with smooth confinement potentials in Hermite functions; confinement potentials are potentials that become unbounded at infinity. The key result is that such eigenfunctions and all their derivatives decay more rapidly than any exponential function under some mild growth conditions to the potential and its derivatives. Their expansion in Hermite functions converges therefore very fast, super-algebraically.

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1 Introduction

This paper is concerned with the numerical solution of Schrödinger equations with so-called confinement potentials, that is, potentials tending to infinity at infinity. In quantum mechanics, such equations describe the motion of particles in an external field that prevents them from escaping to infinity, that is, confines them to a high probability in a finite region. More precisely, we aim to approximate square integrable eigenfunctions $u : \mathbb{R}^d \to \mathbb{R}$ of a Hamilton operator

$$Hu = -\Delta u + Vu, \tag{1.1}$$

with V an infinitely differentiable potential satisfying the condition

$$\lim_{|x|\to\infty} V(x) = +\infty. \tag{1.2}$$

It is well-known that such operators have a purely discrete, unbounded spectrum consisting of eigenvalues of finite multiplicity. Elliptic regularity theory states that the eigenfunctions are themselves infinitely differentiable. A further condition that we

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need for technical reasons is that the potential cannot become unbounded at infinity too fast: we assume that for every multi-index α, there exists constants $c_\alpha \geq 0$ and $\mu_\alpha \geq 0$ such that the partial derivative $\mathrm{D}^\alpha V$ of the potential satisfies the estimate

$$|(\mathrm{D}^\alpha V)(x)| \leq c_\alpha \mathrm{e}^{\mu_\alpha |x|} \tag{1.3}$$

or, as we say, is exponentially bounded. We further assume that the potential itself does not grow faster than a polynomial. An example of an operator satisfying these conditions is the harmonic oscillator, for which $V(x) = |x|^2$.

The eigenfunctions of the harmonic oscillator are explicitly known and are polynomial multiples of the Gauss function. They and all their derivatives decay more rapidly than any exponential function, with arbitrary decay rate. We will show that the eigenfunctions of the given Hamilton operators share this property with the eigenfunctions of the harmonic oscillator. They behave therefore extremely well, both with respect to their smoothness and with respect to their behavior at infinity. Their expansion into the eigenfunctions of the harmonic oscillator converges therefore very rapidly: the error of the best n-term approximation of the eigenfunctions by linear combinations of eigenfunctions of the harmonic oscillator tends faster to zero than any power of $1/n$, a property called super-algebraic convergence.

2 The speed of decay of the eigenfunctions and their derivatives

We begin studying the regularity of the square integrable eigenfunctions of the Hamilton operator (1.1) and the decay behavior of their derivatives. Our proofs are based on arguments similar to those in the monograph [1] of Agmon, in which the decay of Schrödinger type eigenfunctions is studied in much detail. Main result is Theorem 2.1 which states that the eigenfunctions indeed largely behave like the eigenfunctions of the harmonic oscillator. In addition to the assumptions above, we assume that the potential V is strictly positive. This does not represent a restriction as the eigenfunctions are not affected by adding a constant to V. Our first two lemmata fix the functional analytic setting and serve to reformulate the eigenvalue problem in weak form:

Lemma 2.1 *Let f be a given square integrable function and let the infinitely differentiable, square integrable function u solve the differential equation*

$$-\Delta u + Vu - \lambda u = f. \tag{2.1}$$

The function u can then, in terms of its L_2-norm and that of f, be estimated as follows:

$$\int |\nabla u|^2 \,\mathrm{d}x + \int V u^2 \,\mathrm{d}x \leq \|f\|_0 \|u\|_0 + \lambda \|u\|_0^2. \tag{2.2}$$

Proof We first introduce the function $\chi : \mathrm{R}^d \to [0,1]$ by $\chi(x) = (1-r^2)^2$ for $0 \leq r < 1$ and $\chi(x) = 0$ for $r \geq 1$, where $r = |x|$, and set $\chi_\varepsilon(x) = \chi(\varepsilon x)$ for $0 < \varepsilon < 1/4$. Then

$$\int \chi_\varepsilon |\nabla u|^2 \,\mathrm{d}x + \int \chi_\varepsilon V u^2 \,\mathrm{d}x = \int \chi_\varepsilon f u \,\mathrm{d}x + \lambda \int \chi_\varepsilon u^2 \,\mathrm{d}x - \int u \nabla \chi_\varepsilon \cdot \nabla u \,\mathrm{d}x,$$

as can be shown multiplying the equation (2.1) with the continuously differentiable function $\chi_\varepsilon u$ and integrating by parts. As $\chi_\varepsilon(x)^{-1}|(\nabla\chi_\varepsilon)(x)|^2 \leq 16\varepsilon^2$ for $|x| < 1/\varepsilon$ and $(\nabla\chi_\varepsilon)(x) = 0$ otherwise, the third term on the right hand side can be estimated as

$$-\int u\nabla\chi_\varepsilon\cdot\nabla u\,\mathrm{d}x \;\leq\; 2\varepsilon\int u^2\,\mathrm{d}x \,+\, 2\varepsilon\int\chi_\varepsilon|\nabla u|^2\,\mathrm{d}x,$$

which follows from the Cauchy-Schwarz inequality and the estimate $2ab \leq a^2 + b^2$. Inserting this into the equation above and using $0 \leq \chi_\varepsilon \leq 1$, one obtains

$$\int\chi_\varepsilon|\nabla u|^2\,\mathrm{d}x + \int\chi_\varepsilon V u^2\,\mathrm{d}x \;\leq\; \frac{1}{1-2\varepsilon}\,\big\{\,\|f\|_0\|u\|_0 + (\lambda+2\varepsilon)\|u\|_0^2\,\big\}.$$

The left hand side of this estimate thus remains bounded uniformly in ε.The proposition follows with the monotone convergence theorem letting ε tend to zero. □

In other words, the norm given by the expression

$$\|u\|^2 \,=\, \int|\nabla u|^2\,\mathrm{d}x + \int V u^2\,\mathrm{d}x \tag{2.3}$$

of the solutions under consideration of the differential equation (2.1) remains finite. The natural solution space of our eigenvalue problem is the completion of the space of the infinitely differentiable functions with compact support under this norm.

Lemma 2.2 *Every infinitely differentiable function u with finite norm (2.3) can, in the sense of this norm, be approximated arbitrarily well by infinitely differentiable functions with compact support, that is, is contained in the given complete space.*

Proof The idea is again to multiply u with a sequence of appropriately chosen cut-off functions. Let χ be an infinitely differentiable function that takes the values $\chi(x) = 1$ for $|x| \leq 1$ and $\chi(x) = 0$ for$|x| \geq 2$ and set, for $\varepsilon > 0$, $\chi_\varepsilon(x) = \chi(\varepsilon x)$. Then

$$\|u - \chi_\varepsilon u\|^2 \,=\, \int\Big\{|(1-\chi_\varepsilon)\nabla u - u\nabla\chi_\varepsilon|^2 + (1-\chi_\varepsilon)^2 V u^2\Big\}\,\mathrm{d}x.$$

Since $1-\chi_\varepsilon$ and $\nabla\chi_\varepsilon$ are uniformly bounded in ε and tend pointwise to zero for ε going to zero, the proposition follows from the dominated convergence theorem. □

The norm (2.3) is induced by the bilinear form

$$a(u,v) \,=\, \int\Big\{\nabla u\cdot\nabla v + Vuv\Big\}\,\mathrm{d}x \tag{2.4}$$

defined on the completion of the space of the infinitely differentiable functions with compact support under this norm. Since the potential V is by assumption strictly positive, this norm dominates the L_2-norm. From the two lemmas we can therefore deduce that the solutions under consideration of the equation (2.1) satisfy the equation

$$a(u,v) - \lambda(u,v) \,=\, (f,v) \tag{2.5}$$

for all test functions v in this space, that is, are in this sense weak solutions of the equation (2.1). This holds particularly for the case of a vanishing right hand side f, which means that the square integrable classical solutions u of the eigenvalue problem

$$-\Delta u + Vu = \lambda u \tag{2.6}$$

are weak solutions in the given Hilbert space, that is, satisfy the relation

$$a(u,v) = \lambda(u,v) \tag{2.7}$$

for all test functions v in this space. We need these properties to prove the following key result, where our argumentation essentially follows the lines given in [1]. A similar proof for the exponential decay of the eigenfunctions of the electronic Schrödinger equation, with Coulomb potentials, can be found in [7].

Lemma 2.3 *Let f be a given function that decreases in the L_2-sense more rapidly than any exponential function, and let u be an infinitely differentiable, square integrable function that solves the differential equation (2.1). The function u decreases then in the L_2-sense more rapidly than any exponential function, that is, the functions*

$$x \to \mathrm{e}^{\mu|x|}u(x) \tag{2.8}$$

are square integrable for all constants $\mu > 0$.

Proof We first choose an arbitrary $\mu > 0$ and introduce the bounded functions

$$\delta(x) = \mu \, \frac{|x|}{1+\varepsilon\,|x|},$$

with $\varepsilon > 0$ given arbitrarily. Since $|(\nabla\delta)(x)| \leq \mu$ for all $x \neq 0$ and since

$$\nabla(\mathrm{e}^{-\delta}v)\cdot\nabla(\mathrm{e}^{\delta}v) = \nabla v\cdot\nabla v - |\nabla\delta|^2 v^2,$$

we obtain the estimate

$$a(\mathrm{e}^{-\delta}v,\mathrm{e}^{\delta}v) \geq a(v,v) - \mu^2\|v\|_0^2 \geq \int Vv^2\,\mathrm{d}x - \mu^2\|v\|_0^2$$

for the infinitely differentiable functions v that have a compact support and that vanish on a neighborhood of the origin. Next we choose a radius $R > 0$ such that

$$V(x) \geq \mu^2 + \lambda + 1$$

holds for all x outside the ball of radius R around the origin. For functions v that are infinitely differentiable, have a compact support, and vanish on this ball, then

$$\|v\|_0^2 \leq a(\mathrm{e}^{-\delta}v,\mathrm{e}^{\delta}v) - \lambda\,\|v\|_0^2. \tag{2.9}$$

Next, we fix an infinitely differentiable function $\chi : \mathbb{R}^d \to [0,1]$ that takes the values $\chi(x) = 0$ for $|x| \leq R$ and $\chi(x) = 1$ for $|x| \geq R+1$. Let u be an infinitely differentiable function with compact support. Setting $v = \chi\mathrm{e}^{\delta}u$, the estimate (2.9) then becomes

$$\|\chi\mathrm{e}^{\delta}u\|_0^2 \leq a(\chi u,\chi\mathrm{e}^{2\delta}u) - \lambda(\chi\mathrm{e}^{\delta}u,\chi\mathrm{e}^{\delta}u). \tag{2.10}$$

To shift the factor χ to the right hand side, we introduce the function

$$\eta = 2\chi\nabla\chi\cdot\nabla\delta + |\nabla\chi|^2$$

that takes the value $\eta(x) = 0$ for $|x| \le R$ and $|x| \ge R+1$. With help of the relation

$$\nabla(\chi u)\cdot\nabla(\chi \mathrm{e}^{2\delta}u) = \nabla u\cdot\nabla(\chi^2\mathrm{e}^{2\delta}u) + \eta\,\mathrm{e}^{2\delta}u^2,$$

the estimate (2.10) can then be rewritten as

$$\|\chi\mathrm{e}^{\delta}u\|_0^2 \le a(u,\chi^2\mathrm{e}^{2\delta}u) - \lambda(u,\chi^2\mathrm{e}^{2\delta}u) + (u,\eta\,\mathrm{e}^{2\delta}u). \tag{2.11}$$

As $\chi\mathrm{e}^{\delta}$ is a bounded function with bounded first-order partial derivatives and as $\eta\,\mathrm{e}^{2\delta}$ is bounded, this estimate transfers to every function u that can in the sense of the norm induced by the bilinear form (2.4) be approximated arbitrarily well by infinitely differentiable functions with compact support. By Lemma 2.1 and Lemma 2.2, this holds particularly for the square integrable, infinitely differentiable solutions of the differential equation (2.1). Since these solutions satisfy the weak form (2.5) of the differential equation, the estimate (2.11) reduces for them to

$$\|\chi\mathrm{e}^{\delta}u\|_0^2 \le (f,\chi^2\mathrm{e}^{2\delta}u) + (u,\eta\,\mathrm{e}^{2\delta}u) \le \|\mathrm{e}^{2\delta}f\|_0\|u\|_0 + \|\eta\,\mathrm{e}^{2\delta}u\|_0\|u\|_0.$$

Since the functions $\eta\,\mathrm{e}^{2\delta}$ are uniformly bounded in ε and the weighted L_2-norm of f is bounded by the by assumption finite expression

$$\|\mathrm{e}^{2\delta}f\|_0^2 \le \int \mathrm{e}^{4\mu|x|}|f(x)|^2\,\mathrm{d}x,$$

the monotone convergence theorem shows, letting ε tend to zero, that the function

$$x \to \mathrm{e}^{\mu|x|}u(x)$$

is square integrable for the given μ and, as μ was arbitrary, for all $\mu > 0$. □

The lemma particularly implies that the square integrable eigenfunctions of the differential operator (1.1) decay in the L_2-sense more rapidly than any exponential function. This holds without any special assumption on the growth of the potential; the only condition that enters into the proof is that it tends to infinity at infinity. However, to show that the partial derivatives of the eigenfunctions behave correspondingly, we must be able to bound the growth of the potential and of its partial derivatives of arbitrary order by exponential functions and need the assumption (1.3).

Theorem 2.1 *Let $u \in L_2$ be an infinitely differentiable solution of the equation*

$$-\Delta u + Vu = \lambda u. \tag{2.12}$$

Then all partial derivatives of u are square integrable as well and moreover decrease, like the solution itself, in the L_2-sense more rapidly than any exponential function.

Proof The function u itself is by assumption square integrable and decreases, by Lemma 2.3, in the L_2-sense more rapidly than any exponential function. To proceed to the next differentiation order, we observe that the first-order partial derivatives of u are, by Lemma 2.1, square integrable and moreover satisfy the differential equation

$$-\Delta \mathrm{D}_k u + V \mathrm{D}_k u - \lambda \mathrm{D}_k u = -(\mathrm{D}_k V) u.$$

Since the partial derivatives of V are by assumption exponentially bounded and u decreases in the L_2-sense more rapidly than any exponential function, the functions $f = -(\mathrm{D}_k V)u$ belong also to this class. Lemma 2.3 therefore guarantees that the $\mathrm{D}_k u$ decrease in the L_2-sense more rapidly than any exponential function. In the same way one can, differentiating the equation again and again, step from one differentiation order to the next and finish the proof by induction on the differentiation order. □

We end this section with a remark on the dependence of the eigenvalues on the potential. Starting point is their min-max characterization. Let $u_1, u_2 \ldots$ be pairwise orthogonal eigenfunctions for the eigenvalues $\lambda_1 \leq \lambda_2 \leq \ldots$ of the operator (1.1). Then

$$\lambda_m = \min_{\mathscr{V}_m} \max_{v \in \mathscr{V}_m} \frac{a(v,v)}{(v,v)}, \tag{2.13}$$

where the minimum is taken over all m-dimensional subspaces $\mathscr{V}_m$ of the solution space and the maximum, without explicitly stating this, over all $v \neq 0$ in $\mathscr{V}_m$. If we replace the potential V with a potential $\widetilde{V} \geq V$ the eigenvalues increase. Choosing the space $\mathscr{V}_m$ spanned by the eigenfunctions $u_1, \ldots, u_m$ of the original operator to obtain an upper bound for the m-th eigenvalue of the modified operator, we get

$$\lambda_m \leq \widetilde{\lambda}_m \leq \lambda_m + \max_v \int (\widetilde{V} - V)\, v^2 \,\mathrm{d}x, \tag{2.14}$$

where the maximum on the right hand side is taken over all normed functions $v \in \mathscr{V}_m$. This estimate can be easily quantified. Taking into account the decay properties of the eigenfunctions, it demonstrates that the eigenvalues are only marginally affected even by large modifications of the potential that are in a sufficient distance from the origin.

3 Hermite spectral approximation

Theorem 2.1 states that the square integrable eigenfunctions of the Hamilton operator (1.1) are ideally suited for spectral approximation. In this section, we discuss a particular method of this type, the expansion of square integrable functions into a series of eigenfunctions of the quantum harmonic oscillator

$$H\psi = -\frac{1}{2}\Delta\psi + \frac{1}{2}|x|^2\psi \tag{3.1}$$

and discuss the convergence behavior of such expansions. The factor $1/2$ comes from the quantum-mechanical background of the operator and helps in the given context to scale its eigenvalues and the norms introduced below properly.

An orthonormal set of eigenfunctions of the one-dimensional counterpart of the operator (3.1), the Hermite functions φ_n, can be recursively calculated as follows:

$$\varphi_0(x) = \Big(\frac{1}{\pi}\Big)^{1/4} \mathrm{e}^{-x^2/2}, \quad \varphi_{n+1} = \frac{1}{\sqrt{2n+2}}\Big(-\frac{\mathrm{d}}{\mathrm{d}x} + x\Big)\varphi_n. \tag{3.2}$$

The Hermite functions are polynomial multiples

$$\varphi_n(x) = \gamma_n^{-1/2} H_n(x)\,\mathrm{e}^{-x^2/2}, \quad \gamma_n = 2^n n! \sqrt{\pi}, \tag{3.3}$$

of the Gauss function; the polynomial H_n is the Hermite polynomial of order n. The corresponding eigenvalues are $n+1/2$. The Hermite functions form a complete set, that is, every square integrable function can be expanded into an L_2-convergent series of Hermite functions. The one-dimensional harmonic oscillator and with that the Hermite functions are discussed in almost every introductory text to quantum mechanics. We refer to [7] for a mathematically oriented presentation.

As the functions φ_n form an orthonormal basis for $L_2(\mathbb{R})$, their tensor products

$$\phi_\mu(x) = \varphi_{\mu_1}(x_1) \cdot \ldots \cdot \varphi_{\mu_d}(x_d) \tag{3.4}$$

form an orthonormal basis for $L_2(\mathbb{R}^d)$, where μ ranges over all multi-indices μ with nonnegative integer components μ_i. These tensor products are eigenfunctions of the d-dimensional Hamilton operator (3.1) for the eigenvalues

$$\eta_\mu = (\mu_1 + \ldots + \mu_d) + d/2. \tag{3.5}$$

The eigenvalues are therefore degenerate in the multi-dimensional case. Our aim in this section is to discuss the speed of convergence of the orthogonal expansion

$$u = \sum_\mu (u, \phi_\mu)\,\phi_\mu \tag{3.6}$$

of square integrable functions $u : \mathbb{R}^d \to \mathbb{R}$ into a series of these eigenfunctions. The L_2-norm of such a function reads in terms of this orthogonal expansion

$$\|u\|_0^2 = \sum_\mu (u, \phi_\mu)^2. \tag{3.7}$$

We will consider in particular rapidly decreasing functions, functions that, including all their partial derivatives, decrease at infinity more rapidly than every polynomial grows. We measure their smoothness and decay in terms of the norms

$$|||u|||_s = \|H^s u\|_0, \tag{3.8}$$

where H is the Hamilton operator (3.1) and s a nonnegative integer value. The key observation is that these norms can be rewritten in terms of the expansion (3.6) as

$$|||u|||_s^2 = \sum_\mu \eta_\mu^{2s} (u, \phi_\mu)^2, \tag{3.9}$$

the reason being that for rapidly decreasing functions u

$$(H^s u, \phi_\mu) = (u, H^s \phi_\mu) = \eta_\mu^s (u, \phi_\mu). \tag{3.10}$$

To show this, it suffices to restrict oneself to the case $s = 1$. If u has compact support (3.10) then follows integrating by parts. The general case is treated similarly as in the proof of Lemma 2.2 approximating u by functions with compact support. The relation (3.9) can be used to extend the definition of the norms to arbitrary real values s. It implies the following estimate for the speed of convergence:

Theorem 3.1 *For all natural numbers $N = 1, 2, \ldots$ let*

$$P_N u \;=\; \sum_{\eta_\mu < N} (u, \phi_\mu)\, \phi_\mu \tag{3.11}$$

be the L_2-orthogonal projection of a function $u \in L_2$ onto the space spanned by the eigenfunctions for eigenvalues $\eta_\mu < N$. For all rapidly decreasing functions u then

$$|||u - P_N u|||_s \;\leq\; \left(\frac{1}{n}\right)^{\frac{t-s}{d}} |||u|||_t \tag{3.12}$$

in terms of the dimension n of this space, where s and $t > s$ are arbitrary.

Proof As follows from the representation (3.9) of the norms,

$$|||u - P_N u|||_s \;\leq\; N^{s-t}\, |||u|||_t\,.$$

The proposition follows therefore from the crude estimate

$$n \;=\; \#\{\, \mu \,|\, (\mu_1 + \ldots + \mu_d) + d/2 < N \,\} \leq N^d$$

for the dimension of the subspace under consideration. □

The smoothness parameter t can be chosen arbitrarily large for rapidly decreasing functions. The projection error $u - P_N u$ tends therefore in each of the norms (3.8) faster to zero than any negative power of the dimension n of the space spanned by the corresponding eigenfunctions. This effect is independent of the space dimension d. The square integrable eigenfunctions of the Hamilton operator (1.1) fall by Theorem 2.1 into the considered class. The expansion (3.6) of such eigenfunctions into Hermite functions converges therefore asymptotically very fast, super-algebraically.

The convergence theory of the Ritz-Galerkin method for the approximate calculation of the eigenvalues and eigenfunctions of the operator (1.1) is based on approximation error estimates in the energy norm (2.3) induced by the bilinear form (2.4) underlying the eigenvalue problem. We show next that this energy norm can be bounded by a norm (3.8). At this place the assumption that the potential V does not grow faster than a polynomial enters. The basic estimate from which we start is:

Lemma 3.1 *For all infinitely differentiable functions v with compact support and all nonnegative integers k,*

$$\|r^{2k+2}v\|_0^2 \leq 4\,\|r^{2k}Hv\|_0^2 + (4k+2)(4k+d)\|r^{2k}v\|_0^2, \tag{3.13}$$

where H is the differential operator (3.1) and r the euclidean norm of the argument x.

Proof The definition (3.1) of H leads immediately to the representation

$$4\,\|r^{2k}Hv\|_0^2 \,=\, \|r^{2k}\Delta v\|_0^2 - 2\,(r^{4k+2}v,\Delta v) + \|r^{2k+2}v\|_0^2.$$

Integration by parts yields

$$(r^{4k+2}v,\Delta v) \,=\, -(4k+2)(r^{4k}xv,\nabla v) - (r^{4k+2}\nabla v,\nabla v).$$

Once more integrating by parts one obtains

$$(r^{4k}xv,\nabla v) \,=\, -(4k+d)(r^{4k}v,v) - (r^{4k}xv,\nabla v)$$

or, resolving for the left hand side,

$$(r^{4k}xv,\nabla v) \,=\, -\frac{4k+d}{2}\,(r^{4k}v,v).$$

Inserting these relations above, one recognizes that the expression

$$\|r^{2k+2}v\|_0^2 + 2\,\|r^{2k+1}\nabla v\|_0^2 + \|r^{2k}\Delta v\|_0^2$$

is equal to the right hand side of (3.13), which implies the proposition. □

Theorem 3.2 *For all rapidly decreasing functions u and all natural numbers k,*

$$\|r^{2k}u\|_0^2 \,\le\, \sum_\mu \theta(k,\mu)\,\widetilde{\eta}_\mu^{2k}(u,\phi_\mu)^2, \quad \|\Delta^k u\|_0^2 \,\le\, \sum_\mu \theta(k,\mu)\,\widetilde{\eta}_\mu^{2k}(u,\phi_\mu)^2, \tag{3.14}$$

where $\widetilde{\eta}_\mu = 2\eta_\mu$ *has been set and the* $\theta(k,\mu)$ *tend to one as* $|\mu|$ *goes to infinity.*

Proof We state first that the estimate (3.13) holds not only for infinitely differentiable functions with compact support but also for rapidly decreasing functions, as can be seen by approximating these correspondingly. We set $\widetilde{H} = 2H$ and

$$x(k,\ell) \,=\, \|r^{2k}\widetilde{H}^\ell u\|_0^2, \quad c(k) \,=\, (4k+2)(4k+d)$$

for abbreviation. The estimate (3.13) implies then the estimate

$$x(k,\ell) \,\le\, x(k-1,\ell+1) + c(k-1)\,x(k-1,\ell)$$

that holds for the integers $k = 1,2,\dots$ and $\ell = 0,1,2,\dots$ and leads to

$$x(k,\ell) \,\le\, x(0,k+\ell) + \sum_{\nu=1}^{k} c(k-\nu)\,x(k-\nu,\ell+\nu-1).$$

By induction on $m = k+\ell = 0,1,2,\dots$ one finally obtains the estimate

$$x(k,\ell) \,\le\, \sum_{j=0}^{k+\ell} \alpha(k,\ell,j)\,x(0,j),$$

where the $\alpha(k,m-k,j)$, $j,k = 0,\dots,m$, are defined by recursion on m. The recursion starts with $\alpha(0,0,0) = 1$ and continues for $k = 1,\dots,m$ and $j = 0,\dots,m-1$ with

$$\alpha(k,m-k,j) \,=\, \sum_{\nu=1}^{k} c(k-\nu)\,\alpha(k-\nu,m-k+\nu-1,j).$$

The remaining values are $\alpha(k, m-k, m) = 1$ for $k = 0, 1, \ldots, m$ and $\alpha(0, m, j) = 0$ for the indices $j = 0, \ldots, m-1$. In particular we obtain the estimate

$$\|r^{2k}u\|_0^2 \;\le\; \|\widetilde{H}^k u\|_0^2 + \sum_{j=0}^{k-1} \alpha(k,0,j)\, \|\widetilde{H}^j u\|_0^2,$$

or, in terms of the expansion (3.8), (3.9), the first estimate in (3.14), where

$$\theta(k,\mu) \,=\, 1 + \sum_{j=0}^{k-1} \alpha(k,0,j)\, \widetilde{\eta}_\mu^{\,2j-2k}.$$

As the Fourier transformation F maps the rapidly decreasing functions bijectively to the rapidly decreasing functions, as it preserves the L_2-inner product, as it commutes with the operator H and therefore also with the L_2-orthogonal projections onto the eigenspaces of H, and as the Fourier transform of Δu is $(F\Delta u)(\omega) = -|\omega|^2(Fu)(\omega)$, the two estimates (3.14) are completely equivalent and follow from each other. □

We remark that the estimates (3.14) can be extended by interpolation to arbitrary nonnegative exponents but will not make use of that. Theorem 3.2 states that every polynomially weighted L_2-norm and every L_2-like Sobolev norm is dominated by a norm (3.8). This means super-algebraic convergence of $P_N u$ to u in every such norm for every rapidly decreasing function u, and therefore super-algebraic convergence of $P_N u$ to u in the energy norm (2.3) for the eigenfunctions u of the operator (1.1), since the potential V is by assumption bounded by a polynomial. This guarantees super-algebraic convergence of the approximate eigenvalues and eigenfunctions computed with the Ritz-Galerkin method to their continuous counterparts; see [7] for a discussion of the convergence properties of the Ritz-Galerkin method.

It is not difficult to switch to another lengthscale and to expand square integrable functions in the same way as before into the orthonormal eigenfunctions

$$\widetilde{\phi}_\mu(x) \,=\, \omega^{d/4}\phi_\mu(\sqrt{\omega}x) \tag{3.15}$$

for the eigenvalues $\widetilde{\eta}_\mu = \omega\eta_\mu$ of the rescaled operator

$$\widetilde{H}\psi \,=\, -\frac{1}{2}\Delta\psi + \frac{\omega^2}{2}|x|^2\psi \tag{3.16}$$

to adapt them better to the functions under consideration. The qualitative behavior of the expansion does not change under this transformation.

We end with a remark on the calculation of the inner products (2.4)

$$a(u,v) \,=\, \int \big\{\nabla u\cdot\nabla v + |x|^2 uv\big\}\,\mathrm{d}x + \int \{V - |x|^2\} uv\,\mathrm{d}x \tag{3.17}$$

that play an important role in the Ritz-Galerkin method. If u is an eigenfunction of the harmonic oscillator for the eigenvalue η, that is, of the operator (3.1),

$$a(u,v) \,=\, 2\eta \int uv\,\mathrm{d}x + \int \{V - |x|^2\} uv\,\mathrm{d}x, \tag{3.18}$$

an observation that often considerably simplifies the computations.

4 Radially-symmetric potentials

We restrict ourselves now to the three-dimensional case and operators (1.1) with radially symmetric potentials $x \to V(r)$, $r = |x|$. The key observation is that such operators are separable in polar coordinates: every eigenfunction can be expressed as a linear combination of eigenfunctions of the form

$$u(r,\varphi,\vartheta) = r^{-1} f(r) Y_\ell^m(\varphi,\vartheta), \quad r > 0,\ 0 \le \varphi < 2\pi,\ |\vartheta| \le \pi/2, \tag{4.1}$$

where the Y_ℓ^m, $\ell = 0,1,\ldots$, $m = -\ell,\ldots,\ell$, are the normed spherical harmonics. Furthermore the radial parts f vanish at the origin and satisfy the radial equation

$$-f''(r) + \frac{\ell(\ell+1)}{r^2} f(r) + V(r) f(r) = \lambda f(r), \quad r > 0, \tag{4.2}$$

where λ is the eigenvalue in (2.6) for the eigenfunction (4.1) and ℓ is degree of the spherical harmonic appearing in this decomposition. For a careful discussion of the radial Schrödinger equation, and of the radial-angular decomposition of functions on the three-dimensional space in general, we refer again to [7].

Not only do eigenfunctions of the operator of interest admit such a decomposition, but so do the eigenfunctions of the harmonic oscillator into which we expanded them in the previous section. Functions of the form (4.1) with different angular parts Y_ℓ^m are L_2-orthogonal to each other. Therefore only the eigenfunctions of the harmonic oscillator with the same angular part contribute to the expansion of a given eigenfunction (4.1) of the operator (1.1) and need to be taken into account. The problem of approximating the eigenfunctions of the operator (1.1) thus reduces in the given case to the problem of approximating their radial parts by the radial parts of the corresponding eigenfunctions of the harmonic oscillator. The L_2-inner product of two functions u and v of the form (4.1) with the same angular part Y_ℓ^m and radial parts f and g turns into the L_2-inner product of f and g, and their inner product (2.4) into

$$a(u,v) = \int_0^\infty \left(f'(r)g'(r) + \frac{\ell(\ell+1)}{r^2} f(r)g(r) + V(r)f(r)g(r) \right) \mathrm{d}r \tag{4.3}$$

The super-algebraic convergence remains unaffected by this decomposition of the single eigenspaces and formal reduction to one-dimensional subproblems. Through the smaller approximation spaces the convergence speed even increases.

The radial components of the eigenfunctions of the harmonic oscillator are described in many texts on quantum mechanics; for instance [2] develops them in hypergeometric functions. For completeness we give a brief description. The radial components of the eigenfunctions for the eigenvalue λ satisfy the equation

$$\frac{1}{2}\left(-f'' + \frac{\ell(\ell+1)}{r^2} f \right) + \frac{1}{2} r^2 f = \lambda f \tag{4.4}$$

on the interval $r > 0$ and vanish at the origin. The functions

$$\varphi_n(r) = \gamma_n^{-1} r^{\ell+1} L_n^{(\alpha)}(r^2)\,\mathrm{e}^{-r^2/2}, \quad \alpha = \ell + 1/2, \tag{4.5}$$

built up from the Laguerre polynomials $L_n^{(\alpha)}$ with the normalization factors given by

$$\gamma_n^2 = \frac{\Gamma(n+\alpha+1)}{2n!}, \tag{4.6}$$

are solutions of this equation for the eigenvalues

$$\lambda = 2n+\ell+\frac{3}{2}, \quad n = 0,1,2,\ldots, \tag{4.7}$$

and form an L_2-orthonormal system over the positive real axis; see [5], Tables 18.3.1 and 18.8.1. As every polynomial multiple of the three-dimensional Gauss function can be written as finite linear combination of functions (4.1) with radial parts (4.5) and as these functions are conversely polynomial multiples of the three-dimensional Gauss function (see [7], for example), a complete set of eigenfunctions is found.

5 Numerical experiments

In this section we report on some preliminary numerical calculations in order to illustrate the fast convergence of the given spectral approximation. We calculate the minimum eigenvalues of operators (1.1) with help of the Ritz-Galerkin method and the eigenfunctions of the harmonic oscillator (3.1) as ansatz functions. We restrict ourselves to the case of rotationally symmetric potentials in three space dimensions and fix the angular part Y_ℓ^m of the eigenfunctions in advance. The problem then reduces to the calculation of the radial parts of the eigenfunctions. Choosing the ansatz space consisting of the eigenfunctions (4.1) of the harmonic oscillator assigned to the first N radial parts (4.5), the Ritz-Galerkin method entails calculating the minimum eigenvalues of the $(N\times N)$-matrix with entries

$$a(\varphi_m,\varphi_n), \quad n = 0,1,\ldots,N-1, \tag{5.1}$$

where $a(f,g)$ here denotes the radial bilinear form on the right hand side of (4.3). Using the observation at the end of Sect. 3, they simplify to

$$a(\varphi_m,\varphi_n) = (4n+2\ell+3)\,\delta_{mn} + \int_0^\infty [V(r)-r^2]\,\varphi_m(r)\varphi_n(r)\,\mathrm{d}r. \tag{5.2}$$

For polynomial potentials of the form,

$$V(r) = \sum_{k=0}^{K} \beta_k r^{2k}, \tag{5.3}$$

assembling the matrix thus requires only calculating moments of the form

$$\int_0^\infty r^{2k}\varphi_m(r)\varphi_n(r)\,\mathrm{d}r = \frac{1}{\gamma_m\gamma_n}\int_0^\infty s^k L_m^{(\alpha)}(s)L_n^{(\alpha)}(s)\,s^\alpha\,\mathrm{e}^{-s}\,\mathrm{d}s \tag{5.4}$$

for indices $0\le n-m\le k$. This is easily done first expanding $s^k L_m^{(\alpha)}(s)$ in Laguerre polynomials and then using the orthogonality of the Laguerre polynomials in the L_2-space with weight function $s^\alpha\,\mathrm{e}^{-s}$, that is, the L_2-orthogonality of the φ_n.

N	$\ell = 0$	$\ell = 1$
10	3.370356837725094812011027856152	5.083453154278464637649723082743
15	3.370356837724959710963971268150	5.083453154277919256126799050771
20	3.370356837724959708816665722286	5.083453154277919221784454010700
25	3.370356837724959708816491294114	5.083453154277919221783788970536
30	3.370356837724959708816491293290	5.083453154277919221783788953023
35	3.370356837724959708816491293289	5.083453154277919221783788953021
40	3.370356837724959708816491293289	5.083453154277919221783788953021
45	3.370356837724959708816491293289	5.083453154277919221783788953021
50	3.370356837724959708816491293289	5.083453154277919221783788953021
55	3.370356837724959708816491293289	5.083453154277919221783788953021
60	3.370356837724959708816491293289	5.083453154277919221783788953021

Table 1 The approximations of the minimum eigenvalues for the polynomial radial potential (5.5)

N	$\ell = 0$	$\ell = 1$
10	3.398081395500957961647580092851	5.155377163743147070792840201218
15	3.398081395452175112921205606740	5.155377163574245059332415049435
20	3.398081395452165919061079921493	5.155377163574086270987769062842
25	3.398081395452165891420811003816	5.155377163574086057803165037467
30	3.398081395452165891373692945192	5.155377163574086057704992057670
35	3.398081395452165891373616454643	5.155377163574086057703790659868
40	3.398081395452165891373615849221	5.155377163574086057703789128389
45	3.398081395452165891373615845544	5.155377163574086057703789093860
50	3.398081395452165891373615845531	5.155377163574086057703789093648
55	3.398081395452165891373615845530	5.155377163574086057703789093647
60	3.398081395452165891373615845530	5.155377163574086057703789093647

Table 2 The approximations of the minimum eigenvalues for the radial potential $V(r) = \cosh(r)$

Table 1 shows the approximations of the minimum eigenvalues for the potential

$$V(r) = 1 + \frac{1}{2}\, r^2 + \frac{1}{24}\, r^4 \tag{5.5}$$

and the values $\ell = 0$ and $\ell = 1$ fixing the angular part. So as to circumvent the possibility that the exponential convergence may be concealed by rounding errors, the matrix entries (5.2) have been calculated exactly with help of the computer algebra program MAPLE and the eigenvalues then computed with an accuracy of 50 decimal digits. The results have been chopped off after the 30th decimal place. The results are compared in Table 2 with the corresponding results for the potential

$$V(r) = \cosh(r) \tag{5.6}$$

that behaves near the origin like the first one but increases more rapidly than any polynomial and is thus not completely covered by our theory. The matrix entries (5.2) cannot be assembled analytically in this case. Due to the smoothness of the integrands, however, they are amenable to numerical quadrature. Adaptive routines from the QUADPACK collection for an arbitrary numerical type are implemented in [4], allowing one to assemble the matrix entries with the same degree of numerical precision as for the other potential. The library [3] implements a numerical type for multiple-precision floating point arithmetic, and the library [6] templates standard LAPACK routines for such a numerical type. The rapid convergence is obvious in both cases, even if it slows down a little bit for the faster increasing potential.

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