On estimates of decay rates for perturbed Schrödinger and Helmholtz type operators ******* Preprint-VERSION ******

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Abstract—**Decay estimates for the electronic density in equations of Schrödinger type as the Helmholtz problem are derived. For radially-symmetric solutions, these decay estimates are improved and made quantitative. Decay results of the elastic field are also recalled. The analytic results are applied to implement a coarsening strategy to numerically solve the Kohn-Sham problem of quantum mechanics for multimillions of atoms. In the framework of Γ-convergence, minimizers of the Rayleigh quotient in the weighted L^2-topology are studied and monotonicity results for the perturbed and the unperturbed eigenvalue problem are established. In one-dimensional case-studies typical properties of the solutions are investigated and non-exponential decay in 1D is demonstrated.**

Keywords: Nonlinear eigenvalue problems, decay estimates, quasi-continuum method, Γ-limit, density functional theory

1 Introduction

In fundamental work by Thomas and Fermi, [22], [7], it was discovered that the electronic structure of solids in their ground states can be formulated solely in terms of their electron density ρ. This was the foundation of the celebrated Density-Functional Theory (DFT), introduced by Hohenberg and Kohn, [12], [17]. Based on work by Kohn and Sham, [16], the ground state energy in the presence of an external potential v can be obtained by minimizing the energy

$$E(\rho) = F_H(\rho) + F_{XC}(\rho) + F_s(\rho) + \int_\Omega v(x)\rho(x)\,\mathrm{d}x.$$

In this expression, $F_H(\rho)$ describes the electrostatic or *Hartree* energy between electrons, given as the convolution integral

$$F_H(\rho) := \frac{1}{2}\int_\Omega\int_\Omega \frac{\rho(x)\rho(y)}{\|x-y\|}\,\mathrm{d}x\,\mathrm{d}y,$$

$F_{XC}(\rho)$ describes the *exchange and correlation* energy, often stated within the local density approximation (LDA), [17], [16]. Finally, F_s is the kinetic energy of a system of non-interacting electrons with density ρ. If N denotes the number of electrons in the system, the exact computation of the Kohn-Sham kinetic energy requires the computation of N non-interacting electron orbitals, which amounts to solving a system of N coupled Schrödinger equations. To be consistent with the ideas of the Thomas-Fermi ansatz, it is advantageous to represent the kinetic energy solely as a functional of ρ. Several such approximations have been proposed in what is called now the Orbital-Free Density Functional Theory (OFDFT). One prominent example is the *Thomas-Fermi-von Weizäcker*-formulation, [26],

$$F_s(\rho) = \frac{1}{8}\int_\Omega \frac{|\nabla\rho(x)|^2}{\rho(x)}\,\mathrm{d}x + C_{TF}\int_\Omega \rho(x)^{5/3}\,\mathrm{d}x + F_{WT}(\rho),$$

with the Thomas-Fermi constant $C_{TF} = 0.3(2\pi^2)^{1/3}$ and the *Wang and Teter correction* [25],

$$\begin{aligned} F_{WT}(\rho) \;=\; & -\frac{32}{25}C_{TF}\int_\Omega \rho(x)^{5/3} \\ & +0.8C_{TF}\int_\Omega \rho(x)^{5/6}K_{WT}(x) * \rho(x)^{5/6}\,\mathrm{d}x, \end{aligned}$$

where K_{WT} is the Wang-Teter convolution kernel.

In [9], a real-space formulation was derived to solve the orbital-free formulation of quantum mechanics for non-periodic structures. In [10], the quasi-continuum method was applied to solve these equations for millions of atoms. The algorithm is based on a coarse-graining strategy of the numerical mesh away from the local defect. OFDFT yields good results for simple metals, but fails already for covalent bonds. Therefore, in this article we are interested in a numerical solution strategy for the Kohn-Sham problem that works as efficiently as the one documented in [10] for the OFDFT case.

To this end we derive analytic estimates of the decay rate of perturbations to the electron density ρ caused by local defects. These are used later to estimate the numerical error when cutting the long tail of the perturbations to the wave functions caused by the local defects.

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The Kohn-Sham problem amounts to solving the eigenvalue problem

$$\big[-\frac{h}{2m}\triangle + V_{ion}(r) + V_H(r) + V_{XC}\big]\psi_i(r) = \varepsilon_i\psi_i(r),$$

where ψ_i is the i-th wave function of electronic state i and ε_i is the eigenvalue (energy state) of the system.

This article is organized as follows. In Section 2 we formulate the Helmholtz problem that will serve us as a model problem. In Section 3 we recall the class of functions K_d and summarize some well-established theorems on the eigenfunctions and the eigenvalues of the Helmholtz problem. In Section 4 we derive the exponential decay of perturbations of eigenfunctions for $\Omega = \mathbb{R}^3$, also for the periodic case. In the subsequent section 5 we discuss the radially symmetric case where Ω is a ball around 0. By introducing spherical coordinates, we simplify to a system of ordinary differential equations. This is studied explicitly for $V(r) = r^{-1}$ and $V(r) = r^{-2}$ which are the two relevant limiting cases of physical significance.

In Section 6 the minimizers of the Rayleigh functional are investigated in the framework of Γ-convergence and the weighted $L^2(\Omega)$-norm. Section 7 summarizes some known decay results about the elastic field which are also essential for the numerics. In Section 8, the numerical coarse-graining strategy for the Kohn-Sham problem is presented. We end with practical numerical examples that demonstrate that the decay of the integral kernel is necessary for the decay of perturbations to the eigenfunctions.

2 Statement of the problem

If $\Omega \subset \mathbb{R}^d$ is a bounded domain, we are interested in the behavior of eigenvalues and eigenfunctions of the problem

$$\begin{aligned} [-\triangle + V_\varepsilon(x)]u^\varepsilon(x) &= \lambda^\varepsilon u^\varepsilon(x) \quad \text{in } \Omega, && (1)\\ u^\varepsilon(x) &= 0 \quad \text{on } \partial\Omega. && (2)\end{aligned}$$

The term $V_\varepsilon(x)$ represents a potential with small support (depending on ε) that originates from a localized point defect. In the case that Ω is unbounded, one is tempted to replace (2) by

$$\lim_{\|x\|\to\infty} u^\varepsilon(x) = 0. \qquad (3)$$

Below we will show that in many cases the condition (3) is automatically satisfied by the solution and need not be imposed.

As $H^\varepsilon := -\triangle + V_\varepsilon$ is symmetric, any eigenvalue λ^ε in (1) is real. We assume that V_ε is well-behaved such that the operator H_ε has a spectrum of the form

$$\sigma(H_\varepsilon) = \sigma_c(H_\varepsilon) \cup \sigma_p(H_\varepsilon).$$

Here, $\sigma_c(H_\varepsilon)$ is the *continuous spectrum.* For bounded domains Ω we have $\sigma_c(H_\varepsilon) = \emptyset$, for $\Omega = \mathbb{R}^3$ it holds $\sigma_c(H_\varepsilon) = [0,\infty]$. We are interested in the *point spectrum* $\sigma_p(H_\varepsilon) = \{\lambda_j^\varepsilon \,|\, j \in \mathbb{N}\}$ of the operator H_ε located below $\sigma_c(H_\varepsilon)$. The eigenfunctions corresponding to λ_j^ε will be denoted by u_j^ε. The fact that $\sigma_p(H_\varepsilon)$ consists of the negative eigenvalues is shown in [6] by a monotonicity argument comparing to the eigenvalues in the unit ball similar to the proof of Theorem 13 below.

3 The Rayleigh functional and fundamental properties of the eigenfunctions

Definition 1 *A measurable function $V : \mathbb{R}^d \to \mathbb{R}$ is said to lie in K^d if*

(a) for $d \geq 3$

$$\lim_{\alpha\to 0}\Big[\sup_{x\in\mathbb{R}^d} \int_{|x-y|\leq\alpha} |x-y|^{-(d-2)}|V(y)|\;\mathrm{d}y\Big] = 0;$$

(b) for $d = 2$

$$\lim_{\alpha\to 0}\Big[\sup_{x\in\mathbb{R}^d} \int_{|x-y|\leq\alpha} \ln(|x-y|^{-1})|V(y)|\;\mathrm{d}y\Big] = 0;$$

(c) for $d = 1$

$$\sup_{x\in\mathbb{R}^d} \int_{|x-y|\leq 1} |V(y)|\;\mathrm{d}y < \infty.$$

We say that $V \in K^d_{\mathrm{loc}}$ if $V_{|\overline{B_R(0)}} \in K^d$ for all $R > 0$.

The following is helpful to decide if a potential lies in K^d. For a proof see [3].

Lemma 1 (Characterization of K^d) *(i) If $d_1 \leq d_2$, then $K^{d_1} \subset K^{d_2}$.*

(ii) Let

$$L^p_{\mathrm{unif}} := \Big\{v \;\Big|\; \sup_{x\in\mathbb{R}^d} \int_{|x-y|\leq 1} |v(y)|^p\;\mathrm{d}y < \infty\Big\}.$$

Then $L^p_{\mathrm{unif}} \subset K^d$ if $p > \frac{d}{2}$ (for $d \geq 2$) or if $p = 2$ (for $d = 1$).

Lemma 1 ensures by immediate inspection that the radial symmetric potentials $V(r) = |r|^{-l}$ lie in K^3 for $l < 2$.

The first theorem is a sub-solution estimate. For a proof see [11], [3], [19].

Theorem 1 *Let $V_\varepsilon \in K^d_{\mathrm{loc}}$ and let u^ε be a solution to (1) in the sense of distributions, i.e.*

$$\langle -\triangle\varphi, u^\varepsilon\rangle + \langle (V_\varepsilon - \lambda^\varepsilon)\varphi, u^\varepsilon\rangle = 0 \qquad \text{for all } \varphi \in C_0^\infty(\Omega).$$

Then the following is true.

(i) The function u^ε has a continuous representative in Ω.

(ii) For $x \in \Omega$ and $B_r(x) \subset\subset \Omega$ there is a constant $c = c(\Omega, r, \|V^\varepsilon\|_{K^d})$ with

$$|u^\varepsilon(x)| \le c \int\limits_{|x-y|\le r} |u^\varepsilon(y)| \, \mathrm{d}y. \tag{4}$$

Above, we denoted by $\langle\cdot,\cdot\rangle$ the duality pairing

$$\langle \varphi, \psi\rangle := \int_\Omega \varphi(x)\psi(x)\,\mathrm{d}x.$$

Theorem 1 is helpful to obtain pointwise properties from average estimates on u^ε. If $u^\varepsilon \in L^2(\Omega)$, then by (4) we find that $u^\varepsilon(x)$ satisfies (3).

Theorem 2 (Harnack inequality) *Let $V_\varepsilon \in K^d_{\mathrm{loc}}$ and u^ε be a non-negative function that fulfills $H_\varepsilon(u) = \lambda^\varepsilon u^\varepsilon$ in the sense of distributions. Then for any compact set $M \subset \Omega$ there exists a constant $0 < c < \infty$ with $c = c(\Omega, M, V_\varepsilon)$ such that*

$$c^{-1} \le \frac{u^\varepsilon(x)}{u^\varepsilon(y)} \le c \qquad \text{for all } x, y \in M. \tag{5}$$

For a proof of Theorem 2, see, e.g., [11], [3], [19], [24]. The inequality (5) states in particular that $u^\varepsilon \ge 0$ in Ω implies $u^\varepsilon > 0$.

Let $H^m(\Omega)$ denote the Sobolev space of m-times weakly differentiable functions in $L^2(\Omega)$ and $H^m_0(\Omega)$ be the closure with respect to $\|\cdot\|_{H^m(\Omega)}$ of the infinitely often differentiable functions in Ω with compact support. For $u \in H^1_0(\Omega)$ we introduce the *Rayleigh quotient*

$$F_\varepsilon(u) := \underbrace{\frac{\int_\Omega |\nabla u(x)|^2\,\mathrm{d}x}{\int_\Omega u(x)^2\,\mathrm{d}x}}_{=:F_0(u)} + \frac{\int_\Omega V_\varepsilon(x) u(x)^2\,\mathrm{d}x}{\int_\Omega u(x)^2\,\mathrm{d}x}. \tag{6}$$

The Euler-Lagrange equation to (6) shows that minimizers $u_\varepsilon \in H^1_0(\Omega)$ of F_ε solve (1), (2).

Subsequently we collect basic properties of the minimization problem (6) and its minimizers.

For given $\varepsilon > 0$ the existence of a minimizer in (6) follows from the following theorem which is a consequence of the Banach-Alaoglu compactness theorem in $H^1(\Omega)$ and the Rellich-Kondrakov theorem. For a proof see for instance [27].

Theorem 3 *Let $(u_{\varepsilon,k})_{k\in\mathbb{N}} \subset H^1_0(\Omega)$ be a sequence such that $\|\nabla u_{\varepsilon,k}\|_{L^2}$ is bounded uniformly in k. Then there exists a function $u_\varepsilon \in H^1_0(\Omega)$ such that for a subsequence $u_{\varepsilon,k_l} \to u_\varepsilon$ in $L^2(\Omega)$ and $\nabla u_{\varepsilon,k_l} \rightharpoonup \nabla u_\varepsilon$ in $L^2(\Omega)$ as $l \to \infty$.*

From Theorem 3 we directly conclude that

$$\lambda_1^\varepsilon := \min_{u^\varepsilon \in H^1_0(\Omega)} F_\varepsilon(u^\varepsilon) \tag{7}$$

exists and is the smallest eigenvalue to (1), (2). A minimizer $u_1^\varepsilon := u^\varepsilon$ that does not vanish completely is a first eigenfunction.

If u^ε is a minimizer in (7), so is $|u^\varepsilon|$, and by Theorem 2 it follows that $|u^\varepsilon| > 0$. By continuity, (Theorem 1), either $u^\varepsilon > 0$ or $u^\varepsilon < 0$ in Ω. Therefore, the smallest eigenfunction does not change signs.

There are continuous functions in the Sobolev space $H^1_0(\Omega)$ that are unbounded. The following theorem is thus of importance if the domain Ω is not regular or if V_ε does not fulfill the requirements of Theorem 1.

Theorem 4 *Let Ω be a bounded domain and assume $V(\cdot) \ge 0$. Then the eigenfunctions u_j^ε are bounded,*

$$\sup_{x\in\Omega} |u_j^\varepsilon(x)| < \infty.$$

Proof The proof uses a very interesting technique based on [15], Lemma 5.1.

For simplicity of notation, we set in this proof $u := u_j^\varepsilon$, $\lambda := \lambda_j^\varepsilon$, $V := V_\varepsilon$, and assume that u is positive in some subset of Ω with non-zero measure. For $k \ge 0$ we plug in $\max\{u(x) - k, 0\}$ as a test function in the weak formulation of (1), (2) to find

$$\int\limits_{A_k} (|\nabla u|^2 + V u(u-k))\,\mathrm{d}x = \lambda \int\limits_{A_k} u(u-k)\,\mathrm{d}x, \tag{8}$$

where

$$A_k := \{x \in \Omega \mid u(x) > k\}.$$

It holds $k|A_k| \le \|u\|_{L^1}$ and $|A_k| \to 0$ as $k \to \infty$. When we apply the Poincaré-Sobolev inequality to each component of A_k we get

$$\int\limits_{A_k} (u-k)^2\,\mathrm{d}x \le |A_k|^{\frac{2}{n}} \int\limits_{A_k} |\nabla u|^2\,\mathrm{d}x. \tag{9}$$

The combination of (8) and (9) yields

$$\int\limits_{A_k} (u-k)^2\,\mathrm{d}x + |A_k|^{\frac{2}{n}} \int\limits_{A_k} V u(u-k)\,\mathrm{d}x \le \lambda |A_k|^{\frac{2}{n}} \int\limits_{A_k} u(u-k)\,\mathrm{d}x.$$

For the integral on the right hand side we observe

$$\int\limits_{A_k} u(u-k)\,\mathrm{d}x \le 2\int\limits_{A_k}(u-k)^2\,\mathrm{d}x + 2k\int\limits_{A_k}(u-k)\,\mathrm{d}x, \quad (10)$$

which is an easy consequence of the elementary inequality $u \le 2(u-k)+2k$ which holds on A_k. We arrive at

$$\Big[1-2\lambda|A_k|^{\frac{2}{n}}\Big]\int\limits_{A_k}(u-k)^2\,\mathrm{d}x + |A_k|^{\frac{2}{n}}\int\limits_{A_k} Vu(u-k)\,\mathrm{d}x \le 2k\lambda|A_k|^{\frac{2}{n}}\int\limits_{A_k}(u-k)\,\mathrm{d}x.$$

The second integral on the left is non-negative. For $k \ge k_0 := 2\lambda^{\frac{n}{2}}\|u\|_{L^1}$, the term in brackets $[1-2\lambda|A_k|^{\frac{2}{n}}] \ge \frac{1}{2}$. From the Hölder inequality we also infer

$$\Bigg[\int\limits_{A_k}(u-k)\,\mathrm{d}x\Bigg]^2 \le |A_k|\int\limits_{A_k}(u-k)^2\,\mathrm{d}x.$$

After cancellation of $\int\limits_{A_k}(u-k)\,\mathrm{d}x$ we thus conclude

$$\int\limits_{A_k}(u-k)\,\mathrm{d}x \le 4k\lambda\,|A_k|^{1+\frac{2}{n}}. \quad (11)$$

Estimate (11) is the crucial estimate and we can now apply Lemma 5.1 in [15]. In fact, introducing

$$f(k) := \int\limits_{A_k}(u-k)\,\mathrm{d}x = \int\limits_k^\infty |A_t|\,dt,$$

it holds $f'(k) = -|A_k|$ and consequently we can write (11) as

$$f(k) \le 4k\lambda[-f'(k)]^{1+\frac{2}{n}} \quad (12)$$

whenever $k \ge k_0$. If f is non-negative in the interval $[k_0, k]$, the integration of (12) leads to

$$k^{\frac{2}{n+2}} \le k_0^{\frac{2}{n+2}} + (4\lambda)^{\frac{2}{n+2}}\Big[f(k_0)^{\frac{2}{n+2}} - f(k)^{\frac{2}{n+2}}\Big].$$

Since $f(k_0) \le f(0) = \|u\|_{L^1}$ and $f(k) \ge 0$ on the right hand side, this bounds k and therefore $f(k)$ is zero for large k. The precise estimate is

$$f(k) = 0 \quad \text{for } k \ge 4^{1+n}\lambda^{\frac{n}{2}}\|u\|_{L^1},$$

especially $\operatorname{ess\,sup}_\Omega u$ is bounded by the right hand side of this estimate.

For the estimate of $\operatorname{ess\,inf} u$, we can repeat the above discussion for $-u$. □

Theorem 5 (Higher regularity of eigenfunctions) *Assume that $V_\varepsilon \in C^m(\mathbb{R}^d) \cap L^2(\mathbb{R}^d)$ for some $m \ge 0$. Then any eigenfunction u_j^ε of (1) fulfills*

$$u_j^\varepsilon \in C^{m+2}(\mathbb{R}^d) \cap L^2(\mathbb{R}^d).$$

The proof of Theorem 5 follows directly from standard elliptic regularity theory and the Sobolev embedding theorem.

4 Decay of eigenfunctions and decay of local perturbations in $\mathbb{R}^3$

One possibility to derive decay properties of the eigenfunctions in the L^2 setting is the use of the Agmon metric. The following statements are introduced and proved in [2].

For a given smooth curve γ introduce the length

$$L_j^\varepsilon(\gamma) := \int\limits_0^1 (V^\varepsilon(\gamma(t)) - \lambda_j^\varepsilon)_+^{1/2}\|\dot\gamma\|\,dt,$$

where $\|\cdot\|$ is the Euclidean norm in $\mathbb{R}^d$ and $(z)_+ := \max(z,0)$.

The Agmon metric is given by

$$\rho_j^\varepsilon(x,y) := \inf_{\gamma\in P_{x,y}} L_j^\varepsilon(\gamma),$$

where

$$P_{x,y} := \{\gamma \in AC([0,1];\mathbb{R}^d)\,|\,\gamma(0)=x, \gamma(1)=y\}$$

and AC denotes the space of absolutely continuous functions.

The following integral decay is shown in [2].

Theorem 6 *For V^ε real and continuous, let $H^\varepsilon := -\triangle + V^\varepsilon$ be a closed operator bounded below with $\sigma(H^\varepsilon) \subset \mathbb{R}$. Suppose λ_j^ε is an eigenvalue of H^ε and that* $\operatorname{supp}(\lambda_j^\varepsilon - V^\varepsilon(x))_+$ *is a compact subset of $\mathbb{R}^d$. Let $\psi \in L^2(\mathbb{R}^d)$ be an eigenfunction of H^ε such that $H^\varepsilon\psi = \lambda_j^\varepsilon\psi$. Then, for any $\delta > 0$, there exists a positive constant C_δ such that*

$$\int\limits_{\mathbb{R}^d}\exp(2(1-\delta)\rho_j^\varepsilon(x))|\psi(x)|^2\,\mathrm{d}x \le C_\delta,$$

where $\rho_j^\varepsilon(x) := \rho_j^\varepsilon(x,0)$.

We note that with the regularity of the eigenfunctions we can use this integral decay to obtain pointwise bounds. Proceeding as in the proof of Theorem 4 we can obtain the estimate

$$\max_{x\in B_{1/2}(x_0)}|u_j^\varepsilon(x)| \le C_3\|u_j^\varepsilon\|_{L^1(B_{1/2}(x_0))}$$

for a constant C_3 independent of x_0. This follows by choosing the test function $\max\{u(x)-k,0\}_{|B_{1/2}(x_0)}$, where we now have $A_k = \{x \in B_{1/2}(x_0)\,|\,u(x) > k\}$. So it also holds

$$\max_{x\in B_{1/2}(x_0)}|u_j^\varepsilon(x)| \le C_3\|u_j^\varepsilon\|_{L^2(B_1(x_0))}.$$

So we may compute

$$\begin{aligned}
&\max_{x\in B_{1/2}(x_0)} |u_j^\varepsilon(x)e^x| \\
&\quad\le\; C_3\Big[\max_{x\in B_1(x_0)} e^x\Big]\Big[\max_{y\in B_1(x_0)} e^{-y}\Big]\|u_j^\varepsilon \exp(\cdot)\|_{L^2(B_1(x_0))} \\
&\quad\le\; C_4.
\end{aligned}$$

We have shown

$$|u_j^\varepsilon(x_0)| \le Ce^{-x_0}.$$

As x_0 was arbitrary, the eigenfunction satisfies a pointwise exponential bound. The Agmon metric is in particular a useful tool to derive *anisotropic* estimates.

Next we show how one can derive the exponential decay of u_j^ε in $\mathbb{R}^3$ in a more direct and very natural way using decay properties of the Green's function. For the subsequent theorem it is convenient to make the assumption

$$|V_\varepsilon(x)| \le q(\|x\|), \quad \text{for } x \in \mathbb{R}^3\setminus\{0\} \tag{13}$$

uniformly in $\varepsilon > 0$, and q is a non-negative square-integrable function that fulfills for a positive constant c_0 the growth conditions

$$\begin{aligned}
\lim_{r\to\infty} q(r) &= 0, &(14)\\
\lim_{r\to 0}(rq(r)) &\le c_0. &(15)
\end{aligned}$$

Theorem 7 *Let $V_\varepsilon \in K^3_{\mathrm{loc}}$ fulfill (13)-(15) and let u_j^ε be a solution to (1) for $\Omega = \mathbb{R}^3$ in the sense of distributions. Then, for any $0 < \alpha_j < |\lambda_j^\varepsilon|^{1/2}$, there exists a constant $0 < c_1(\alpha_j) < \infty$ such that for all $x \in \mathbb{R}^3$*

$$|u_j^\varepsilon(x)| \le c_1(\alpha_j)\exp(-\alpha_j\|x\|). \tag{16}$$

Proof The proof exploits the decay properties of the Green's function. The same construction fails for space dimensions $d < 3$.

The key observation is that the eigenfunctions u_j^ε fulfill the integral identity

$$u_j^\varepsilon(x) = \int_{\mathbb{R}^3} \frac{\exp(-|\lambda_j^\varepsilon|^{1/2}\|x-y\|)}{4\pi\|x-y\|} V_\varepsilon(y)u_j^\varepsilon(y)\;\mathrm{d}y. \tag{17}$$

$\Big[$With the abbreviation

$$I(y) := \int_{\mathbb{R}^3} \frac{\exp(-|\lambda_j^\varepsilon|^{1/2}\|x-y\|)}{\|x-y\|}\triangle\varphi(x)\,\mathrm{d}x$$

it holds

$$\begin{aligned}
-4\pi[\triangle u_j^\varepsilon](\varphi) &= -4\pi\int_{\mathbb{R}^3} u_j^\varepsilon(x)\triangle\varphi(x)\,\mathrm{d}x \\
&= -\int_{\mathbb{R}^3} V_\varepsilon(y)u_j^\varepsilon(y)I(y)\;\mathrm{d}y
\end{aligned}$$

and

$$\begin{aligned}
I(y) &= \int_{\mathbb{R}^3} \frac{\exp(-|\lambda_j^\varepsilon|^{1/2}\|x\|)}{\|x\|}\triangle\varphi(x+y)\,\mathrm{d}x \\
&= \int_{\mathbb{R}^3} \Big[\triangle\Big(\frac{\exp(-|\lambda_j^\varepsilon|^{1/2}\|x\|)}{\|x\|}\Big) + \mathrm{div}(\mathcal{N})\Big]\varphi(x+y)\,\mathrm{d}x \\
&= \int_{\mathbb{R}^3} \Big[\frac{-\lambda_j^\varepsilon \exp(-|\lambda_j^\varepsilon|^{1/2}\|x\|)}{\|x\|} \\
&\qquad + \exp(-|\lambda_j^\varepsilon|^{1/2}\|x\|)\triangle\Big(\frac{1}{\|x\|}\Big)\Big]\varphi(x+y)\,\mathrm{d}x.
\end{aligned}$$

Here we used the symbol

$$\begin{aligned}
\mathcal{N} := \exp\big(-|\lambda_j^\varepsilon|^{1/2}\|x\|\big)\nabla(\|x\|^{-1}) \\
-|\lambda_j^\varepsilon|^{1/2}\frac{\exp(-|\lambda_j^\varepsilon|^{1/2}\|x\|)}{\|x\|}.
\end{aligned}$$

As $\Omega = \mathbb{R}^3$ is unbounded we get $\int_{\mathbb{R}^3}\mathrm{div}(\mathcal{N}) = 0$.

Using

$$\begin{aligned}
&\int_{\mathbb{R}^3} \exp(-|\lambda_j^\varepsilon|^{1/2}\|x\|)\triangle\Big(\frac{1}{\|x\|}\Big)\varphi(x+y)\,\mathrm{d}x \\
&\qquad = 4\pi[\delta_y](\varphi) = 4\pi\,\varphi(y)
\end{aligned}$$

this implies

$$-4\pi[\triangle u_j^\varepsilon](\varphi) = 4\pi\lambda_j^\varepsilon[u_j^\varepsilon](\varphi) - 4\pi\int_{\mathbb{R}^3}\varphi(y)V_\varepsilon(y)u_j^\varepsilon(y)\;\mathrm{d}y.\ \Big]$$

With (13), the identity (17) yields

$$|u_j^\varepsilon(x)| \le \int_{\mathbb{R}^3} \frac{\exp(-|\lambda_j^\varepsilon|^{1/2}\|x-y\|)}{4\pi\|x-y\|} q(\|y\|)|u_j^\varepsilon(y)|\;\mathrm{d}y. \tag{18}$$

For $0 < \alpha_j < |\lambda_j^\varepsilon|^{\frac12}$ we introduce the functions

$$\begin{aligned}
p(x) &:= \sup_{y\in\mathbb{R}^3}\big\{|u_j^\varepsilon(y)|\exp(-\alpha_j\|x-y\|)\big\}, \\
G_{\alpha_j}(x) &:= \int_{\mathbb{R}^3} \frac{\exp(-(|\lambda_j^\varepsilon|^{1/2}-\alpha_j)\|x-y\|)}{4\pi\|x-y\|} q(\|y\|)\;\mathrm{d}y.
\end{aligned}$$

The function G_{α_j} is continuous and rotationally invariant. From (18) we infer

$$|u_j^\varepsilon(x)| \le G_{\alpha_j}(x)p(x). \tag{19}$$

We next show that

$$\lim_{\|x\|\to\infty} G_{\alpha_j}(x) = 0. \tag{20}$$

To this end, for a parameter $s > 0$, consider G_{α_j} separately on the two domains

$$\begin{aligned}
I_1(s) &:= \{y \in \mathbb{R}^3 \mid \|x-y\| < s\}, \\
I_2(s) &:= \{y \in \mathbb{R}^3 \mid \|x-y\| > s\}.
\end{aligned}$$

Introducing polar coordinates and exploiting (15) we find for $G_{\alpha_j}(x)$ on $I_1(s)$

$$\begin{aligned}
&\int\limits_{B_s(x)} \frac{\exp(-(|\lambda_j^\varepsilon|^{1/2}-\alpha_j)\|x-y\|)}{4\pi\|x-y\|} q(\|y\|)\,\mathrm{d}y \\
&\leq \frac{C}{\|x\|} \int\limits_0^s \frac{r^2\exp(-(|\lambda_j^\varepsilon|^{1/2}-\alpha_j)r)}{4\pi r} q(r)\,dr \\
&\leq \frac{C}{\|x\|} \int\limits_0^s r\exp(-(|\lambda_j^\varepsilon|^{1/2}-\alpha_j)r) q(r)\,dr \\
&\leq C(c_0)s^2\|x\|^{-1}.
\end{aligned}$$

On $I_2(s)$ we find by direct estimates

$$\begin{aligned}
&\int\limits_{I_2} \frac{\exp(-(|\lambda_j^\varepsilon|^{1/2}-\alpha_j)\|x-y\|)}{4\pi\|x-y\|} q(\|y\|)\,\mathrm{d}y \\
&< \frac{1}{4\pi s}\int\limits_{I_2} \exp(-(|\lambda_j^\varepsilon|^{1/2}-\alpha_j)\|x-y\|) q(\|y\|)\,\mathrm{d}y \\
&\leq \frac{C}{s}\int\limits_{I_2} \exp(-(|\lambda_j^\varepsilon|^{1/2}-\alpha_j)\|z\|)\,dz \\
&\leq \frac{C}{s}\int_{\mathbb{R}^3} \exp(-(|\lambda_j^\varepsilon|^{1/2}-\alpha_j)\|z\|)\,dz,
\end{aligned}$$

where in the second line of this estimate (14) was used.

Choosing $s := \|x\|^{1/4}$ we get that both estimates for $G_{\alpha_j}(x)$ on $I_1(s)$ and on $I_2(s)$ tend to 0 as $\|x\| \to \infty$ which implies (20).

Theorem 1 states that u_j^ε is continuous and decays pointwise to 0 as $\|x\| \to \infty$. Together with (20) it follows that for a sufficiently large $0 < R < \infty$ we have that

$$G_{\alpha_j}(x) < 1 \text{ for all } x \in \mathbb{R}^3 \setminus B_R(0)$$

and that p attains its supremum in $\overline{B_R(0)}$, i.e.

$$p(x) = \max_{y\in\overline{B_R(0)}} \big\{|u_j^\varepsilon(y)|\exp(-\alpha_j\|x-y\|)\big\}. \tag{21}$$

From the boundedness of u_j^ε in $\overline{B_R(0)}$ and from (21) we obtain now directly for a positive constant $c_2 = c_2(R, \alpha_j)$

$$p(x) \leq c_2\exp(-\alpha_j\|x\|) \quad \text{for all } x \in \mathbb{R}^3.$$

The last estimate in combination with (19) and the boundedness of G_{α_j} proves the theorem. ☐

Let u_j^0 denote the j-th eigenfunction to (1), (3) on the whole space with $V \equiv 0$.

Theorem 8 (Exp. decay of perturbations, $\boldsymbol{\Omega=\mathbb{R}^3}$) *Additional to the assumptions of Theorem 7 assume that H_ε is a self-adjoint operator. Then it holds for sufficiently large x*

$$|u_j^\varepsilon(x) - u_j^0(x)| \leq C\exp(-\gamma_j\|x\|)$$

for constants $C > 0$ and $0 < \gamma_j < |\lambda_j^\varepsilon|^{1/2}$.

Proof For u_j^0 we use the explicit representation in [23], p.78f. For $\Omega = \mathbb{R}^k$, $\operatorname{Im}(\sqrt{\lambda_j^0}) > 0$ and $r = \|x\|$ this is

$$u_j^0(r) = r^{1-\frac{k}{2}} C_{kj} H^{(1)}_{\frac{k}{2}-1}\big(r\sqrt{\lambda_j^0}\big), \tag{22}$$

where

$$C_{kj} := i2^{-\frac{k}{2}-1}\pi^{1-\frac{\lambda_j^0}{2}}(\lambda_j^0)^{\frac{k}{4}-\frac{1}{2}}$$

and $H_n^{(1)}(x) := J_n(x)+iY_n(x)$ is the *first Hankel function* (and J_n and Y_n are Bessel functions). The solution given by (22) decays for large $\|x\|$ like $\exp(-|\lambda_j^0|^{1/2}\|x\|)$ since for $z \in \mathbb{C}$ with $\|z\|$ sufficiently large

$$H_n^{(1)}(z) \sim \sqrt{\frac{2}{\pi\|z\|}}\, e^{i\left(z-\frac{\pi}{4}-\frac{n\pi}{2}\right)}, \tag{23}$$

evaluated at the imaginary $z := r|\lambda_j^0|^{1/2}i$ for large r.

In Theorem 7 we have already found that u_j^ε for $\varepsilon > 0$ decays exponentially in $\mathbb{R}^3$. With (23) this proves the theorem. ☐

4.1 The case $\Omega = \mathbb{R}^3$ with periodic potential

Now we consider potentials with periodic contributions, again in $\Omega = \mathbb{R}^3$. We consider the problem

$$[-\triangle + V_\varepsilon(x) + V_\#(x)]u_j^\varepsilon(x) = \lambda_j^\varepsilon u_j^\varepsilon(x) \qquad \text{in } \mathbb{R}^3. \tag{24}$$

In (24), by $V_\#$ we denote a periodic potential (usually with $\int_{\mathbb{R}^3} V_\#(y)\,\mathrm{d}y = 0$) that we assume to be bounded almost everywhere. We can state the following modification of Theorem 8.

Theorem 9 (Decay in $\mathbb{R}^3$ with periodic potential) *Let $V_\varepsilon \in K^3_{\mathrm{loc}}$ fulfill the assumptions (13)-(15) and assume that $V_\# \in L^\infty(\mathbb{R}^3)$ is a periodic potential. Let u_j^ε be an eigenfunction to problem (24) with corresponding eigenvalue λ_j^ε and $0 < \alpha_j < |\lambda_j^\varepsilon|^{1/2}$. Then there exists a constant $c_2 = c_2(\alpha_j) < \infty$ such that for sufficiently large x*

$$|u_j^\varepsilon(x)| \leq c_2(\alpha_j)\exp(-\alpha_j\|x\|). \tag{25}$$

Furthermore, for sufficiently large x, a constant $C > 0$ and any $0 < \gamma_j < |\lambda_j^\varepsilon|^{1/2}$ it holds

$$|u_j^\varepsilon(x) - u_j^0(x)| \leq C\exp(-\gamma_j\|x\|). \tag{26}$$

Proof: As in Theorem 7 we have for any $0 < \alpha_j < |\lambda_j^\varepsilon|^{1/2}$

$$|u_j^\varepsilon(x)| \leq \big[G_{1,\alpha_j}(x) + G_{2,\alpha_j}(x)\big]p(x) \tag{27}$$

with

$$\begin{aligned} p(x) &:= \sup_{y\in\mathbb{R}^3}\Big\{\exp(-\alpha_j\|x-y\|)|u_j^\varepsilon(y)|\Big\}, \\ G_{1,\alpha_j}(x) &:= \int_{\mathbb{R}^3}\frac{\exp(-(|\lambda_j^\varepsilon|^{1/2}-\alpha_j)\|x-y\|)}{4\pi\|x-y\|}q(\|y\|)\ \mathrm{d}y, \\ G_{2,\alpha_j}(x) &:= \left|\int_{\mathbb{R}^3}\frac{\exp(-(|\lambda_j^\varepsilon|^{1/2}-\alpha_j)\|x-y\|)}{4\pi\|x-y\|}V_\#(y)\ \mathrm{d}y\right|. \end{aligned}$$

The functionals G_{1,α_j} and G_{2,α_j} are continuous and rotationally invariant.

Based on the assumptions (13)-(15) we can show exactly as in Theorem 7 that

$$\lim_{\|x\|\to\infty} G_{1,\alpha_j}(x) = 0. \tag{28}$$

From $V_\#\in L^\infty(\mathbb{R}^3)$ we infer for a non-negative constant c

$$\lim_{\|x\|\to\infty} G_{2,\alpha_j}(x) \leq c.$$

In combination with (28), this implies the boundedness of $G_{1,\alpha_j} + G_{2,\alpha_j}$ in $\mathbb{R}^3$.

Lemma 1, (ii) shows that $V_\# \in K^3_{\mathrm{loc}}$, thus Theorem 1 applies, yielding the continuity of u_j^ε and the pointwise convergence $u_j^\varepsilon(x) \to 0$ as $\|x\| \to \infty$.

So we find again for some large enough $R > 0$

$$p(x) = \sup_{y\in\overline{B_R(0)}}\Big\{|u_j^\varepsilon(y)|\exp(-\alpha_j\|x-y\|)\Big\}.$$

With the continuity of u_j^ε, this results directly in

$$p(x) \leq c_3\exp(-\alpha_j\|x\|)$$

for a constant $c_3 > 0$. This proves (25).

Inequality (26) follows since (25) holds also if $V_\varepsilon \equiv 0$ and, by assumption, $u_j^0 \not\equiv 0$. This confirms the exponential decay of u_j^0. □

5 The local decay of perturbations in a bounded, spherical domain

We study (1), (2) by introducing spherical polar coordinates (r,φ,θ) in $\mathbb{R}^3$. We assume that V is radially symmetric, $V(x) = V(r)$, $r = \|x\|_2$, and study the decay properties of perturbations of the solution in $\Omega = B_R(0)$ for given $R > 0$.

The separation ansatz

$$u(r,\varphi,\theta) = u_1(r)u_2(\varphi)u_3(\theta) \tag{29}$$

for the n-th eigenfunction leads to the equation

$$\begin{aligned} &\frac{1}{r^2u_1(r)}\frac{d}{dr}\big(r^2u_1'(r)\big) + \frac{1}{r^2u_2(\varphi)\sin^2\theta}u_2''(\varphi) \\ &+\frac{1}{r^2u_3(\theta)\sin\theta}\frac{d}{d\theta}\big(\sin\theta\, u_3'(\theta)\big) - V(r) = -\lambda_j, \end{aligned}$$

and λ_j is the j-th eigenvalue as before.

We multiply with $r^2\sin^2\theta$ and resolve with respect to $u_2''(\varphi)$ to find

$$\begin{aligned} &\frac{1}{u_2(\varphi)}u_2''(\varphi) \\ &= r^2\sin^2\theta\Big[-\lambda_j + V(r) - \frac{1}{r^2u_1(r)}\frac{d}{dr}\big(r^2u_1'(r)\big) \\ &\qquad -\frac{1}{r^2\sin\theta\, u_3(\theta)}\frac{d}{d\theta}\big(\sin\theta\, u_3'(\theta)\big)\Big]. \end{aligned}$$

The left hand side is a function of φ only, the right hand side is a function of r and θ only. Choosing $-L^2$ as integration constant, we therefore have

$$\frac{1}{u_2(\varphi)}u_2''(\varphi) = -L^2, \tag{30}$$

$$\begin{aligned} &\frac{1}{r^2u_1(r)}\frac{d}{dr}\big(r^2u_1'(r)\big)+\frac{1}{r^2u_3(\theta)\sin\theta}\frac{d}{d\theta}\big(\sin\theta\, u_3'(\theta)\big) \\ &-\frac{L^2}{r^2\sin^2\theta} - V(r) = -\lambda_j. \end{aligned} \tag{31}$$

Multiplication with r^2 and rearrangement leads to

$$\begin{aligned} &\frac{1}{u_1(r)}\frac{d}{dr}\big(r^2u_1'(r)\big) + r^2(\lambda_j - V(r)) \\ &= -\frac{1}{\sin\theta\, u_3(\theta)}\frac{d}{d\theta}\big(\sin\theta\, u_3'(\theta)\big) + \frac{L^2}{\sin^2\theta}. \end{aligned} \tag{32}$$

The separation of (32) yields for a constant b

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\big(\sin\theta\, u_3'(\theta)\big)+\Big(b-\frac{L^2}{\sin^2\theta}\Big)u_3(\theta) = 0, \tag{33}$$

$$\frac{1}{r^2}\frac{d}{dr}\big(r^2u_1'(r)\big)+\big(\lambda_j-V(r)\big)u_1(r)-\frac{b}{r^2}u_1(r) = 0. \tag{34}$$

So we have converted the partial differential equation into the three ordinary differential equations (30), (33) and (34).

For certain $V(r)$ the solutions to (34) can be expressed by Bessel functions, (33) is *Legendre's equation.* Once the solutions u_1, u_2, u_3 have been calculated, the most general solution based on (29) is of the form

$$u_m(r,\varphi,\theta) = \sum_m u_{1,m}(r)u_2(\varphi)u_{3,m}(\theta), \tag{35}$$

where $u_{1,m}(R) = 0$ in order to fulfill the boundary condition (2).

With the substitution $u_{3,m}(\theta) = v_{3,m}(\xi)$ and $\xi = \cos(\theta)$ we obtain

$$\begin{aligned}(1-\xi)^2 \frac{d^2}{d\xi^2} v_{3,m}(\xi) - 2\xi \frac{d}{d\xi} v_{3,m}(\xi) \\ + \Big[m(m+1) - \frac{L^2}{1-\xi^2}\Big] v_{3,m}(\xi) = 0.\end{aligned}$$

The solutions are given by the *associated Legendre polynomials*

$$v_{3,m}(\xi) \equiv P_m^L(\xi) = (1-\xi^2)^{L/2} \frac{d^L}{d\xi^L} P_m(\xi),$$

where

$$P_m(\xi) = \frac{1}{2^m m!} \frac{d^m}{d\xi^m} \Big[(\xi^2-1)^m\Big]$$

is the *Legendre polynomial* of order m.

The remaining key step is the solution of (34). We discuss different solutions depending on the choice of V.

5.1 Decay of the radial solution, $V(r) = r^{-1}$

In (34) it holds $b = m(m+1)$. This originates from the solution of the Legendre equation (33). With $V(r) = r^{-1}$ we therefore have to solve

$$r^2 \tilde{u}_1''(r) + 2r\tilde{u}_1'(r) + [\lambda_j r^2 - r - m(m+1)]\tilde{u}_1(r) = 0.$$

The substitution $\tilde{u}_1(r) = r^m v(r)$ leads to the equation

$$r v''(r) + 2(m+1)v'(r) + [\lambda_j r - 1]v(r) = 0. \tag{36}$$

The unperturbed case $V(r) = 0$ is analogously represented by

$$r w''(r) + 2(m+1)w'(r) + \lambda_j r\, w(r) = 0, \tag{37}$$

where $u_1(r) := r^m w(r)$ solves (34) with $V(r) = 0$.

With the parameters

$$\alpha_m = m+1, \quad \beta_m = 2(m+1), \quad \varrho_j = -2\sqrt{-\lambda_j}r \leq 0$$

the solution to (37) is given by

$$w(r) = \exp\big(\sqrt{-\lambda_j}r\big)\Phi\big(\alpha_m, \beta_m, \varrho_j\big), \tag{38}$$

where $\Phi(\alpha, \beta, \varrho)$ solves the degenerate *hypergeometric equation*

$$\varrho\Phi''(\varrho) + (\beta - \varrho)\Phi'(\varrho) - \alpha\Phi(\varrho) = 0. \tag{39}$$

A particular solution is given by the *Kummer series* representation

$$\Phi(\alpha, \beta, \varrho) = 1 + \sum_{l=1}^{\infty} \frac{(\alpha)_l}{(\beta)_l l!} \varrho^l \tag{40}$$

with $(\alpha)_l := \alpha(\alpha+1) \cdot \ldots \cdot (\alpha + l - 1) = \Gamma(\alpha+l)/\Gamma(\alpha)$ and the general solution to (39) can be constructed with this ansatz (40).

The equations (36) and (37) only differ by one factor, i.e. $(\lambda_j r - 1)$ instead of $\lambda_j r$, so we expect the solutions to be very similar. In fact, proceeding as before, we can verify that the solution to (36) is

$$v(r) = \exp\big(\sqrt{-\lambda_j}r\big)\Phi\big(\alpha_m - \mu_j, \beta_m, \varrho_j\big),$$

with

$$\mu_j := \frac{1}{2\sqrt{-\lambda_j}} > 0$$

and the other parameters $\alpha_m = m+1$, $\beta_m = 2(m+1)$, $\varrho_j = -2\sqrt{-\lambda_j}r$ are unchanged.

For the difference $\tilde{u}_1(r) - u_1(r)$ of the perturbed and the unperturbed solution we compute, summing over all $m \in \mathbb{N}$ as explained in (35)

$$\begin{aligned}|\tilde{u}_1(r) - u_1(r)| = \sum_{m=1}^{\infty} r^m \exp\big(\sqrt{-\lambda_j}r\big) \\ \times \big|\Phi(\alpha_m - \mu_j, \beta_m, \varrho_j) - \Phi(\alpha_m, \beta_m, \varrho_j)\big|.\end{aligned}$$

Using the representation (40) we find

$$\begin{aligned}&\sum_{m=1}^{\infty} r^m \big|\Phi(\alpha_m - \mu_j, \beta_m, \varrho_j) - \Phi(\alpha_m, \beta_m, \varrho_j)\big| \\ &= \sum_{m=1}^{\infty} r^m \sum_{k=1}^{\infty} \frac{|(m+1-\mu_j)_k - (m+1)_k|}{(2m+2)_k} \frac{\varrho_j^k}{k!} \\ &= \sum_{k=1}^{\infty}\sum_{m=1}^{\infty} r^m \Big|\frac{\Gamma(m+1-\mu_j+k)}{\Gamma(m+1-\mu_j)} - \frac{\Gamma(m+1+k)}{\Gamma(m+1)}\Big| \\ &\qquad \times \frac{\Gamma(2m+2)}{\Gamma(2m+2+k)} \frac{\varrho_j^k}{k!} \\ &< \sum_{k=1}^{\infty}\sum_{m=1}^{\infty} r^m \Big|\frac{\Gamma(m+1-\mu_j+k) - \Gamma(m+1+k)}{\Gamma(m+1-\mu_j)}\Big| \\ &\qquad \times \frac{\Gamma(2m+2)}{\Gamma(2m+2+k)} \frac{\varrho_j^k}{k!}.\end{aligned}$$

We can show directly that

$$\begin{aligned}\sum_{m=1}^{\infty} r^m \Big|\frac{\Gamma(m+1-\mu_j+k) - \Gamma(m+1+k)}{\Gamma(m+1-\mu_j)}\Big| \\ \times \frac{\Gamma(2m+2)}{\Gamma(2m+2+k)} \leq C\end{aligned} \tag{41}$$

uniformly in $k \geq 1$. Estimate (41) holds since for fixed k

$$\lim_{m\to\infty} r^m \frac{\Gamma(m+1-\mu_j+k) - \Gamma(m+1+k)}{\Gamma(m+1-\mu_j)} = 0.$$

So we may conclude

$$\begin{aligned}|\tilde{u}_1(r) - u_1(r)| \leq \sum_{m=1}^{\infty} r^m \exp(\sqrt{-\lambda_j}r) \\ \times \big|\Phi(\alpha_m - \mu_j, \beta_m, \varrho_j) - \Phi(\alpha_m, \beta_m, \varrho_j)\big| \\ \leq C\exp(\sqrt{-\lambda_j}r + \varrho_j) = C\exp(-\sqrt{-\lambda_j}r).\end{aligned}$$

Actually, in Estimate (41) we do not exploit that $\mu_j \to 0$ as $j \to \infty$. Consequently, the estimate could be sharpened for large j.

We summarize the result in the following theorem.

Theorem 10 (Decay of perturbed u_j, $\mathbf{V(r) = r^{-1}}$) *Let $\tilde{u}_j$ be an eigenvector to (1), (2) with $V(r) = r^{-1}$ and j-th eigenvalue λ_j in $\Omega = B_R(0)$ that permits the separation ansatz (29). Let u_j be the corresponding eigenvector to the unperturbed problem with $V(r) = 0$, also satisfying (29).*

Then, for the positive constants

$$\begin{aligned} C_j \;=\; & \sup_{\varphi\in[0,2\pi]} |u_2(\varphi)| \sup_{m\in\mathbb{N}} \sup_{\theta\in[0,\pi]} |u_{3,m}(\theta)| \\ & \times \max_{k\geq 1} \Big\{ \sum_{m=1}^{\infty} \Big| \frac{\Gamma(m+1-\mu_j+k) - \Gamma(m+1+k)}{\Gamma(m+1-\mu_j)} \Big| \\ & \qquad\qquad \times \frac{\Gamma(2m+2)}{\Gamma(2m+2+k)} \; R^m \Big\}, \end{aligned}$$

it holds

$$|\tilde{u}_j(r) - u_j(r)| \leq C_j \exp(-|\lambda_j|^{1/2} r). \qquad (42)$$

Remark 1 *(i) Estimate (42) extends the analysis of Theorem 8 to the case of a bounded spherical domain and $V(r) = r^{-1}$ without additional constraints on the radial distance r away from the defect at* 0.

(ii) The unperturbed radial solution $u_1(r)$ has itself exponential decay. This can be read off the Kummer series representation for u_1 noting $\alpha_m < \beta_m$. The argument is made precise in the proof of Theorem 11 below.

(iii) The calculations to Theorem 10 asssumed for simplicity that $\tilde{\lambda}_j = \lambda_j$, ie. that the eigenvalues of the perturbed and the unperturbed systems are identical. The general case can be optained from that computation since both $u_1(r)$ and $\tilde{u}_1(r)$ decay exponentially away from 0. In addition, $|\lambda_j - \tilde{\lambda}_j|$ can be estimated by Theorem 13 below.

5.2 Radial solution for $V(r) = cr^0$

The methods of the previous subsection also allow to investigate the case $V(r) = c$ for a constant $c > 0$. Equality (34) with $V(r) = c$ becomes

$$r^2 \hat{u}_1''(r) + 2r\hat{u}_1' + [(\lambda_j - c)r^2 - b]\hat{u}_1(r) = 0.$$

After the substitution $\hat{u}_1(r) = r^m \hat{w}(r)$ we are led to the ordinary differential equation

$$r\hat{w}''(r) + 2(m+1)\hat{w}'(r) + (\lambda_j - c)r\hat{w}(r) = 0. \qquad (43)$$

The solution to (43) is

$$\hat{w}(r) = \exp(\sqrt{c-\lambda_j}\,r)\Phi(m+1, 2(m+1), -2\sqrt{c-\lambda_j}\,r).$$

We compare the solution $\hat{u}_1(r)$ to the solution $u_1(r)$ of the unperturbed system with $V(r) = 0$ given by (38). Let $\alpha_m := m+1$, $\beta_m := 2(m+1)$ as in the previous section. We estimate

$$\begin{aligned} |u_1(r) - \hat{u}_1(r)| \leq & \sum_{m=1}^{\infty} r^m [\exp(\sqrt{c-\lambda_j}\,r) - \exp(\sqrt{-\lambda_j}\,r)] \\ & \times \Phi(\alpha_m, \beta_m, -2\sqrt{c-\lambda_j}\,r) \\ & + \sum_{m=1}^{\infty} r^m \exp(\sqrt{-\lambda_j}\,r) \\ & \times \big| \Phi(\alpha_m, \beta_m, -2\sqrt{c-\lambda_j}\,r) - \Phi(\alpha_m, \beta_m, -2\sqrt{-\lambda_j}\,r) \big|. \end{aligned} \qquad (44)$$

For estimating the second sum in (44), we observe similar to (41)

$$\begin{aligned} & \sum_{m=1}^{\infty} r^m |\Phi(\alpha_m, \beta_m, -2\sqrt{c-\lambda_j}\,r) - \Phi(\alpha_m, \beta_m, -2\sqrt{-\lambda_j}\,r)| \\ & \quad = \sum_{k=1}^{\infty} \sum_{m=1}^{\infty} r^m \frac{\Gamma(m+1+k)\Gamma(2m+2)}{\Gamma(m+1)\Gamma(2m+2+k)} \\ & \qquad\qquad \times \frac{[-2\sqrt{c-\lambda_j}\,r]^k - [2\sqrt{-\lambda_j}\,r]^k}{k!} \\ & \quad \leq \hat{C}_j \big[\exp(-2\sqrt{c-\lambda_j}\,r) - \exp(-2\sqrt{-\lambda_j}\,r) \big] \end{aligned}$$

for a suitable constant $\hat{C}_j$ specified below similar to the estimate (41). Thus, the second sum in (44) is estimated by

$$\hat{C}_j \exp(-\sqrt{c-\lambda_j}\,r).$$

Analogously we find

$$\sum_{m=1}^{\infty} r^m |\Phi(\alpha_m, \beta_m, -2\sqrt{c-\lambda_j}\,r)| < \hat{C}_j \exp\big(-2\sqrt{c-\lambda_j}\,r\big)$$

and the first sum in (44) is estimated by

$$\hat{C}_j \exp\big(-\sqrt{c-\lambda_j}\,r\big).$$

So we have shown

Theorem 11 (Decay of perturbed u_j for $\mathbf{V(r){=}c}$) *Let $\hat{u}_j$ be an eigenvector to (1), (2) with $V(r) = c$ and j-th eigenvalue λ_j in $\Omega = B_R(0)$ that permits the separation ansatz (29). Let u_j be the corresponding eigenvector to the unperturbed problem with $V(r) = 0$, also satisfying (29).*

Then, for the positive constants

$$\begin{aligned} \hat{C}_j \;=\; & \sup_{\varphi\in[0,2\pi]} |u_2(\varphi)| \sup_{m\in\mathbb{N}} \sup_{\theta\in[0,\pi]} |u_{3,m}(\theta)| \\ & \times \max_{k\geq 1} \Big\{ \sum_{m=1}^{\infty} \frac{\Gamma(m+1+k)\Gamma(2m+2)}{\Gamma(m+1)\Gamma(2m+2+k)} \; R^m \Big\} \end{aligned}$$

it holds

$$|\hat{u}_j(r) - u_j(r)| \leq 2\hat{C}_j \exp(-\sqrt{c-\lambda_j}\,r). \qquad (45)$$

5.3 Radial solution for $V(r) = r^{-2}$

The relevant cases for applications include

$$\frac{A}{r^\alpha} \le V(r) < \frac{B}{r^\beta}$$

with positive constants A and B and $0 \le \beta \le \alpha < 2$. Therefore, the choice $V(r) = r^{-2}$ made here is unphysical and only interesting as a limiting situation. In addition, $V(r) = r^{-2}$ does *not* satisfy the assumption (15) of Theorem 7 and Theorem 8.

Starting from (34) we arrive at

$$r^2 \tilde{\tilde{u}}_1''(r) + 2r\tilde{\tilde{u}}_1'(r) + [\lambda_j r^2 - 1 - m(m+1)]\tilde{\tilde{u}}_1(r) = 0.$$

This ordinary differential equation is well-studied.

With $\nu = \sqrt{m(m+1) + 5/4}$ the general solutions are given by

$$\tilde{\tilde{u}}_1(r) = r^{-1/2}\Big[C_1 J_\nu(\sqrt{\lambda_j}r) + C_2 Y_\nu(\sqrt{\lambda_j}r)\Big] \qquad (46)$$

for arbitrary constants C_1, C_2.

But, in this case, the solution $\tilde{\tilde{u}}_1$ becomes complex and the analysis breaks down.

6 Γ-limit of the Rayleigh functional

For $\alpha > 0$ we introduce the weighted L^2-norm

$$\|u\|_{L^2_\alpha} := \int_\Omega (1 + |x|)^\alpha u(x)^2 \,\mathrm{d}x$$

and

$$L^2_\alpha(\Omega) := \{u \in L^2(\Omega) \mid \|u\|_{L^2_\alpha} < \infty\}.$$

The family of functionals $(F_\varepsilon)_{\varepsilon>0}$ defined on $L^2_\alpha(\Omega)$ with values in $\mathbb{R} \cup \{\infty\}$ is said to Γ-converge for $\varepsilon \searrow 0$ to F_0 for a chosen argument $u \in L^2_\alpha(\Omega)$, if the following two conditions are met:

(i) Let $(u_\varepsilon)_{\varepsilon>0} \subset L^2_\alpha(\Omega)$ be an arbitrary sequence with $\lim_{\varepsilon\searrow 0} \|u_\varepsilon - u\|_{L^2_\alpha} = 0$. Then

$$F_0(u) \le \liminf_{\varepsilon\searrow 0} F_\varepsilon(u_\varepsilon).$$

(ii) There exists a sequence $(u_\varepsilon)_{\varepsilon>0} \subset L^2_\alpha(\Omega)$ such that $\|u_\varepsilon - u\|_{L^2_\alpha} = 0$ and

$$F(u) \ge \limsup_{\varepsilon\searrow 0} F_\varepsilon(u_\varepsilon).$$

The convergence $\|u_\varepsilon - u\|_{L^2_\alpha} \to 0$ implies for $\alpha \ge 2$ the convergence of the areas.

The subsequent Theorem is the main theorem of Γ-convergence. For a proof see for instance [5].

Theorem 12 (Minimum property of the Γ-limit) *Suppose that u^ε is a minimizer of F_ε in $L^2_\alpha(\Omega)$ and $u^\varepsilon \to u^0$ in $L^2_\alpha(\Omega)$ as $\varepsilon \searrow 0$. If F_ε additionally Γ-converges for fixed $u^0 \in L^2_\alpha(\Omega)$ to F_0 as $\varepsilon \searrow 0$, then u^0 is a minimizer of F_0 and*

$$\lim_{\varepsilon\searrow 0} F_\varepsilon(u^\varepsilon) = F_0(u^0).$$

To demonstrate the strength of the Γ-convergence technique, we study the limit behavior of localized potentials in three dimensions that satisfy the assumptions

$$\begin{aligned} |\mathrm{supp}\, V_\varepsilon| &= C\varepsilon, & (47)\\ \|V_\varepsilon u\|_{L^2} &\le q\|\nabla u\|_{L^2} & (48) \end{aligned}$$

for some $q > 0$ and small $\varepsilon > 0$.

We recall the definition (6) of the Rayleigh quotient. From this definition and (47) we get that $(F_\varepsilon)_{\varepsilon>0}$ is a monotonically decreasing sequence. Therefore we get directly $\Gamma - \lim_{\varepsilon\searrow 0} F_\varepsilon = F_0$. In connection with Theorem 12 this tells us that the family of eigenfunctions $(u_1^\varepsilon)_{\varepsilon>0}$ to the smallest eigenvalue λ_1^ε converges uniformly to the eigenfunction u_1^0 of the linear eigenvalue problem, i.e. to (1), (2) with $V \equiv 0$.

For the analysis of the eigenvalues λ_j^ε for $j > 1$, we require for the rest of this section that F_ε is *even*, that is $F_\varepsilon(u) = F_\varepsilon(-u)$ for every $u \in H^1_0(\Omega)$.

The estimate of the eigenvalues λ_j^ε, $j \ge 2$ requires an additional tool, the *Krasnoselskii genus*. Subsequently we shortly introduce this concept, but refer to [21] and [4] for a more complete presentation.

We call a set $S \subset H^1_0(\Omega)$ *symmetric with respect to the origin* if $v \in S$ implies $-v \in S$. The *Krasnoselskii genus* $\gamma(S)$ is defined as the smallest number $j \in \mathbb{N}$ such that there exists a continuous odd mapping $\Phi : S \to \mathbb{R}^j \setminus \{0\}$. If no such mapping Φ exists, we set $\gamma(S) := +\infty$. In particular, if $0 \in S$, then $\gamma(S) = +\infty$, as $\Phi(0) = 0$ for any odd mapping Φ. If Φ exists, then it holds $\Phi(v) = -\Phi(-v)$ for any $v \in S$.

Let S_j denote the collection of all subsets $S \in H^1_0(\Omega)$, symmetric with respect to the origin, such that $\gamma(S) \ge j$ and the set $\{v \in S \mid \|v\|_{L^2} = 1\}$ is compact.

As shown in [21], the Palais-Smale theory yields that

$$\lambda_j^\varepsilon := \inf_{S\in S_j} \max_{u\in S} F_\varepsilon(u) \qquad (49)$$

is a critical value of F_ε. From the Euler-Lagrange equation it follows as before that λ_j^ε is an eigenvalue of (1), (2).

Due to the monotonicity of F_ε the Γ-limit of F_ε can be easily computed as before, now restricted to the set S_j.

We summarize the results in the following

Theorem 13 *Let F_ε be an even functional. Suppose that V_ε satisfies (47), (48). Then it holds for every $j \in \mathbb{N}$:*

(i) The eigenfunction u_j^ε minimizes the Rayleigh quotient among all functions in $S_j \subset H_0^1(\Omega)$. A minimizer to the first eigenfunction does not change sign.

(ii) The family of eigenvalues $(\lambda_j^\varepsilon)_{\varepsilon>0}$ of (1), (2) converges for $\varepsilon \searrow 0$ to the eigenvalue λ_j^0 of the linear eigenvalue problem.

(iii) The eigenvector u_j^ε to the eigenvalue λ_j^ε is a minimizer of F_ε in $S_j \subset H_0^1(\Omega)$ and converges in the strong topology of $L^2_\alpha(\Omega)$ to the eigenvector u_j^0 of the linear eigenvalue problem.

(iv) $\lambda_j^\varepsilon \geq \lambda_j^0, \qquad \lambda_j^\varepsilon \leq \lambda_j^0 + q\varepsilon$.

Remark 2 *By the 2. Poincaré inequality (or by Hardy's inequality), Condition (48) is satisfied for $V(r) = 1/r$, since for any $v \in C_0^\infty(\Omega)$*

$$\left\| \frac{v(\cdot)}{|\cdot|} \right\|_{L^2} \leq 2 \|\nabla v\|_{L^2}.$$

Proof (i)-(iii) have been shown above.

(iv) Fix $j \in \mathbb{N}$ and let $S \in S_j$, $u \in S$. With (49) the estimate $F_\varepsilon \geq F_0$ yields directly $\lambda_j^\varepsilon \geq \lambda_j^0$. The estimate $\lambda_j^\varepsilon \leq \lambda_j^0 + q\varepsilon$ follows from (49) with the decomposition

$$F_\varepsilon(u) = F_0(u) + \frac{\int_\Omega V_\varepsilon(x) u^2(x)\,\mathrm{d}x}{\int_\Omega u^2(x)\,\mathrm{d}x}$$

and the assumptions (47), (48). □

7 Decay estimates for the elastic field

We shortly summarize some results about the decay estimates of the elastic field. This is needed later for the numerical implementation. The results are taken from the review articles [13], [14].

Theorem 14 *Let R be a cylinder in $\mathbb{R}^3$ of length $l > 0$ whose cross section is bounded. Let $u \in C^2(\overline{R})$ be the solution of the elasticity problem*

$$\operatorname{div}(\nabla u) = 0 \qquad \text{in } \overline{R},$$

subject to the boundary conditions

$$\frac{\partial}{\partial x_1} u(0, x_2) \;=\; f(x_2), \quad \frac{\partial}{\partial x_1} u(l, x_2) = 0,$$

Then it holds for a constants K, M_0, and $\mu_1 > 0$

$$|u(x_1, x_2, x_3)| \leq K M_0 \exp(-\mu_1 x_3), \quad 0 \leq x_3 \leq l,$$

where the x_3-coordinate runs parallel to the generators of the cylinder. The constant μ_1 can be determined by solving an eigenvalue problem and it holds $\mu_1 l \gg 1$.

8 A coarsening strategy for the numerical solution of the Kohn-Sham problem with millions of atoms

In [20], a non-periodic finite element formulation of the Kohn-Sham problem of quantum mechanics was formulated. In [10], an orbital-free formulation was solved numerically for millions of atoms, relying on a coarse-graining strategy of the numerical mesh away from the local defects. In case of the Kohn-Sham problem, this objective is non-trivial, since the wave functions must be computed which is non-trivial. Based on the estimates found in the preceding parts of this article, we subsequently derive and present a coarse-graining strategy for the Kohn-Sham problem which works as efficiently as in [10]. [...]

9 Decay of perturbations in a bounded one-dimensional interval

Theorem 7 shows exponential decay for eigenfunctions to problem (1), (3) in $\mathbb{R}^3$. Its proof fails for space dimensions smaller than 3 as then the Green's function does not have suitable decay properties. A natural question is whether this is a shortcoming of the mathematical proof or whether the decay properties in these space dimensions are actually not good enough. In this subsection we answer this question for $d = 1$.

For given $L > 0$, we solve (1), (2) numerically, subdividing the domain $\Omega = (0, L) \subset \mathbb{R}$ equidistantly with discretization points $x_i = ih$, $1 \leq i \leq N$ for small $h > 0$. The second derivative $\frac{d^2}{dx^2}\psi$ is resolved with a central difference quotient. The eigenvalues and eigenfunctions of the resulting discrete system are computed with the Linear Algebra PACKage LAPACK, see `www.netlib.org/lapack/`.

For $V(x) \equiv 0$, the solutions are given by the *Bloch waves*

$$\psi_l(x) = \sin(\pi * l * x/L), \quad l \in \mathbb{N}.$$

In our numerical studies, we set $L = 10$.

For the first test we choose

$$V(x) = V_1(x) := M_1 \mathcal{X}_B(x)$$

with $M_1 := 256$ and $B := B_{0.1}(5)$. Figure 1 shows the first 16 eigenfunctions for $h = 1/64000$ and V (truncated, as M_1 is too large).

First we notice that in accordance to Theorem 2, the smallest two eigenfunctions do not change sign. Next

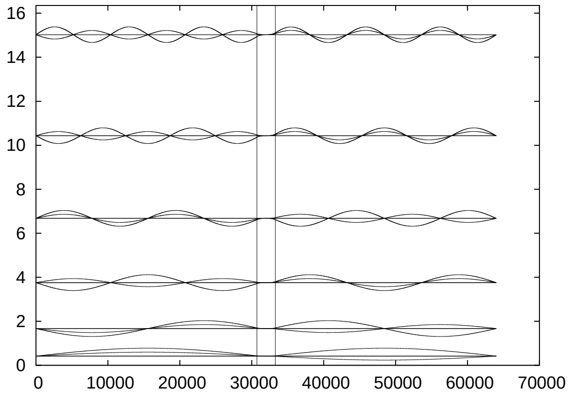

Figure 1: Eigenfunctions in 1-d for $V = V_1$

we observe that the eigenfunctions are approximately 0 in $B \subset \Omega$ where V_1 is large. This perfectly agrees with Theorem 13, as any eigenfunction u is a minimizer of the Rayleigh quotient. Notice also that the zeros of the eigenfunctions near B are not exactly on ∂B, as the term $\int_\Omega |\nabla u|^2$ contributes to the Rayleigh quotient.

As B is located exactly at the center of Ω, the problem of Figure 1 is symmetric and this symmetry is reflected in the eigenfunctions, revealing pairs of u_j with only the sign changed. This is a frequently encountered case in quantum mechanics. Figure 2 displays what happens when we shift B to the left.

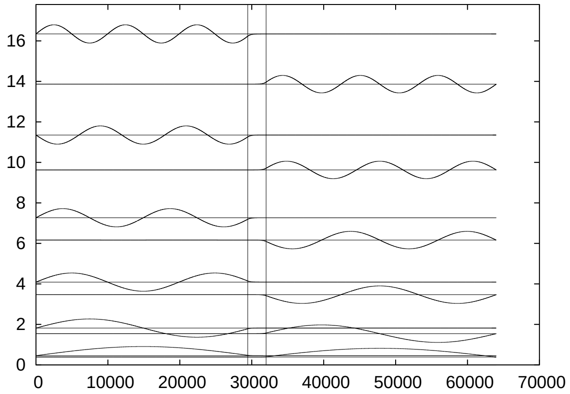

Figure 2: Eigenfunctions in 1-d for shifted potential V_1

Finally, the following Figure 3 documents the effect of M on the eigenfunctions. We set $M := 320$ and observe as explained above only a moderate effect on the eigenfunctions. Also, in Figure 3 we increased the resolution to $h = 1/80000$ to improve the quality of the output.

Most importantly, all the computed results show that there is no exponential decay of the eigenfunctions away from the defect around B. This makes clear that the statements of Theorem 7 cannot be generalized to $\mathbb{R}^1$.

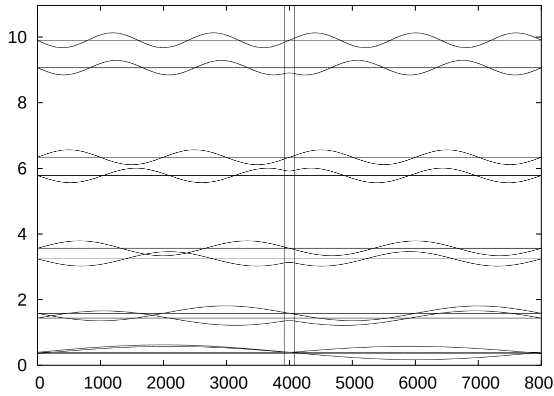

Figure 3: Influence of M on the eigenfunctions

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