

A REVIEW OF FINITE APPROXIMATIONS, ARCHIMEDEAN AND NON-ARCHIMEDEAN

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ABSTRACT. We give a review of finite approximations of quantum systems, both in an Archimedean and a Non-Archimedean setting. Proofs will generally be omitted. In the Appendix we present some numerical results.

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1. INTRODUCTION

An early result in the topic of finite approximations of quantum systems was published in a joint paper by Varadarajan, Varadhan and myself in 1994 [DVV94]. The underlying space was d -dimensional Euclidean space \mathbf{R}^d , and the Hamiltonian $H = -\Delta + V$ was acting in $L^2(\mathbf{R}^d)$; here Δ is the the Laplacian and the potential V is a multiplication operator: $(Vf)(x) = v(x)f(x)$, where v is a non-negative, continuous function such that $v(x) \rightarrow \infty$ as $|x| \rightarrow \infty$. The latter condition ensures that H has a discrete spectrum. Appropriate finite models were set up, and under

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various conditions it was shown that the eigenvalues and eigenfunctions of the finite models converged to the corresponding objects of H (in a certain precise sense). Two proofs were given: a standard functional analytic one, and a stochastic one. In the latter a stronger convergence result was obtained: eigenfunctions were shown to converge uniformly on compacta (and not just in the L^2 -norm). A quick review of these results is given in Section 2.

The next step was to do for quantum systems over local fields what had been done for quantum systems over \mathbf{R}^d . This was accomplished in a couple of articles some twenty years later [BD15, BDW17]. Again two methods of proof were employed: standard functional analytic [BD15] and stochastic [BDW17]; the latter gave, as above, a sharper convergence result for the eigenfunctions. These results are reviewed in Section 3.

The above results have been extended to a setting of locally compact abelian groups in [AGK00]. However, the proofs used non-standard analysis, and will not be commented on here.

All the above works dealt with Hamiltonians with discrete spectrum. The problem of obtaining similar results for Hamiltonians with mixed spectrum was attacked by Erik M. Bakken in his PhD thesis [Bak16]. Here the setting was that of a Hamiltonian with atomic potential in \mathbf{R}^3 : $H = -\Delta + V$ acts in $L^2(\mathbf{R}^3)$ where $(Vf)(x, y, z) = v(r)f(x, y, z)$, $v(r) = -1/r$, $r = \sqrt{x^2 + y^2 + z^2}$. The approximation is done in two steps: one first approximates within a finite box, and then lets the box grow to fill up the whole space \mathbf{R}^3 , in such a way that the approximating grid gets finer and finer and, at the same time, goes to infinity with the box. A quick review of these results is given in Section 4.

In the Appendix we present some numerical results, illustrating the accuracy of the finite models.

2. FINITE APPROXIMATIONS OVER THE REALS

We give a summary of the results in [DVV94]. The setting is as follows:

Hamiltonian. $H = -\Delta + V$ acts in $L^2(\mathbf{R}^d)$, where Δ is the d -dimensional Laplacian, and the potential V is given as $(Vf)(x) = v(x)f(x)$, where $v \geq 0$ is continuous and $v(x) \rightarrow \infty$ as $|x| \rightarrow \infty$.

Finite model. The finite models which were discussed can be divided into two main types: one where the Laplacian is defined via the finite difference operator, and one where the Laplacian is defined via the multiplication operator and the finite Fourier transform. The latter is referred to as the Schwinger model.

Let $\epsilon > 0$ and denote by $G(\epsilon)$ the lattice $(\mathbf{Z}\epsilon)^d \subset \mathbf{R}^d$. For $h \in G(\epsilon)$ the translation operator T_h acts on functions on $G(\epsilon)$ by $(T_h f)(x) = f(x + h)$, $x \in G(\epsilon)$.

Finite difference model. . If e_i , $i = 1 \dots d$, are the standard basis vectors in \mathbf{R}^d , the partial difference operators $D_i(\epsilon)^\pm$ are defined by

$$D_i(\epsilon)^+ = \epsilon^{-1}(T_{\epsilon e_i} - I), \quad D_i(\epsilon)^- = \epsilon^{-1}(I - T_{-\epsilon e_i}) \quad i = 1 \dots d$$

and the discrete Laplacian $\Delta(\epsilon)$ by

$$\Delta(\epsilon) = \sum_{1 \leq i \leq d} D_i(\epsilon)^- D_i(\epsilon)^+$$

The Hamiltonian $H(\epsilon)$ on $L^2(G(\epsilon))$ is given by $H(\epsilon) = -\Delta(\epsilon) + V_\epsilon$, where the operator V_ϵ acts as multiplication by the restriction of v to $G(\epsilon)$. To get to the finite level one introduces a natural number $N^0 = N^0(\epsilon)$ depending on ϵ such that $\epsilon N^0 \rightarrow \infty$ as $\epsilon \rightarrow 0$, and sets $N = N(\epsilon) = 2N^0 + 1$. $G(\epsilon)^0$ is the subgrid $X(\epsilon)^d$ of $G(\epsilon)$ where $X(\epsilon) = \{r\epsilon \mid r = 0, \pm 1, \dots, \pm N^0\}$. One now needs to restrict the

discrete Laplacian $\Delta(\epsilon)$ to the finite grid $G(\epsilon)^0$, and this can be done in several ways, depending on the treatment of boundary conditions. One can use periodic boundary conditions; the corresponding operators are then given a superscript (p) : $H(\epsilon)^{(p)} = -\Delta(\epsilon)^{(p)} + V_\epsilon$. Another class of boundary conditions is also described in [DVV94], and the corresponding operators are marked with superscript (0) : $H(\epsilon)^{(0)} = -\Delta(\epsilon)^{(0)} + V_\epsilon$. A simple example from the latter class is obtained by setting $\Delta(\epsilon)^{(0)} = P_\epsilon \Delta(\epsilon) P_\epsilon$, where P_ϵ is multiplication by the characteristic function of $G(\epsilon)^0$ and $L^2(G(\epsilon)^0)$ is identified with a subspace of $L^2(G(\epsilon))$ in the obvious way.

Schwinger model. As in the periodic case the finite grid $G(\epsilon)^0$ is now identified with $G(\epsilon)/(N(\epsilon) \cdot G(\epsilon))$, a finite group with N^d elements. The associated finite Fourier transform is denoted by \mathcal{F}_ϵ . We also fix the relationship between ϵ and N : $\epsilon = \sqrt{2\pi/N}$. Differentiation at the finite level is now defined, not by the finite difference operator, but by the finite Fourier transform of the multiplication operator, in analogy with the relation at the continuous level: $p := \frac{1}{i} \frac{d}{dx} = \mathcal{F}^{-1} q \mathcal{F}$, where \mathcal{F} is the Fourier transform and q is multiplication by the coordinate: $(qf)(x) = xf(x)$. So we define, for $i = 1 \dots d$:

$$(q_{i,\epsilon} f)(x) = x_i f(x) \quad (x \in G(\epsilon)), \quad p_{i,\epsilon} = \mathcal{F}_\epsilon^{-1} q_{i,\epsilon} \mathcal{F}_\epsilon, \quad -\Delta(\epsilon)^{(s)} = \sum_{1 \leq i \leq d} p_{i,\epsilon}^2$$

$$H^{(s)}(\epsilon) = -\Delta(\epsilon)^{(s)} + V_\epsilon.$$

Imbedding of finite model into $L^2(\mathbf{R}^d)$, and convergence. Finally we need to define an isometric imbedding of $L^2(G(\epsilon))$ (and hence also of $L^2(G(\epsilon)^0)$) into $L^2(\mathbf{R}^d)$. We first define, for each $x \in \mathbf{R}^d$

$$R(x) = \{y = (y_1, \dots, y_d) \mid x_i - \epsilon/2 \leq y_i < x_i + \epsilon/2\}$$

and then define the isometric imbedding $f \in L^2(G(\epsilon)) \mapsto f^\# \in L^2(\mathbf{R}^d)$ by

$$f^\# = \epsilon^{-d/2} \sum_{x \in G(\epsilon)} f(x) \chi_{R(x)} \quad (\chi_E: \text{characteristic function of } E).$$

Via this imbedding operators on $L^2(G(\epsilon))$ can be thought of as operators on $L^2(\mathbf{R}^d)$ in the obvious way.

After considerable effort the main result of [DVV94] was stated as follows

Theorem 2.1 (Theorem 4 in [DVV94]). *Let (ϵ_n) be a sequence tending to 0 and $* = p, s, 0$. Let $0 < h_1 < h_2 < \dots$ be the eigenvalues of H and T_j the eigenspace corresponding to h_j . Then (i) if J is a compact subset of $[0, \infty)$ not containing any eigenvalues of H , then no eigenvalue of $H(\epsilon_n)^{(*)}$ belongs to J if n is large enough; (ii) if J is a compact neighborhood of h_j not containing any h_i , $i \neq j$, all the eigenvalues of $H(\epsilon_n)^{(*)}$ that belong to J converge to h_j ; if T_{n_j} is the span of the corresponding eigenspaces, $\dim(T_{n_j}) = \dim(T_j)$ for n large enough, and there is an orthonormal basis of T_{n_j} that converges to an orthonormal basis of T_j .*

This theorem was proved both by standard analytic and stochastic methods. The two methods of proof will be commented on in the non-Archimedean section, where similar methods are used. *The stochastic method* allowed for a stronger conclusion, namely that the eigenvectors converged not only in the L^2 -norm, but also in the topology of *uniform convergence on compacta*.

3. FINITE APPROXIMATIONS OVER A LOCAL FIELD

3.1. Quick facts about local fields. We give here some quick facts about local fields. For a thorough treatment, see the classic treatise of A. Weil [Wei74, Ch. I]; for a quicker review, see the book of Kochubei [Koc01a, Ch. 1.3].

A local field is a non-discrete, locally compact field. The only connected local fields are \mathbf{R} and \mathbf{C} . Disconnected local fields are, in fact, totally disconnected.

Every local field comes equipped with a canonical absolute value which defines its topology. It is induced by the Haar measure and is called *module* in [Wei74]. It is Archimedean in the case of \mathbf{R} and \mathbf{C} , and non-Archimedean in all other cases; it coincides with the usual absolute values for the fields \mathbf{R} , \mathbf{C} , and \mathbf{Q}_p . For a general local field K we will denote the canonical absolute value by $|\cdot|$.

Convention. Since all local fields except \mathbf{R} and \mathbf{C} are (totally) disconnected, it is customary to reserve the term 'local field' for a (totally) disconnected, non-discrete, locally compact field. We will follow that convention here.

With this convention, there are two main types of local fields:

Characteristic zero. The basic example of a local field of characteristic zero is the p -adic field \mathbf{Q}_p (p a prime number). Every local field of characteristic zero is a finite extension of \mathbf{Q}_p for some p .

Positive characteristic. Every local field of positive characteristic p is isomorphic to the field $\mathbf{F}_q((t))$ of Laurent series over a finite field \mathbf{F}_q , where $q = p^f$ for some positive integer $f \geq 1$.

Let K be a local field with canonical absolute value $|\cdot|$. Following standard notation, we set

$$O = \{x \in K : |x| \leq 1\}, \quad P = \{x \in K : |x| < 1\}, \quad U = O \setminus P.$$

O is a compact subring of K , called the *ring of integers*. It is a discrete valuation ring, i.e., a principal ideal domain with a unique maximal ideal. P is the unique non-zero maximal ideal of O , called the *prime ideal*, and any element $\beta \in P$ such that $P = \beta O$ is called a *uniformizer* (or a *prime element*) of K . For \mathbf{Q}_p one can choose $\beta = p$, and for $\mathbf{F}_q((t))$ one can take $\beta = t$.

The set U coincides with the *group of units* of O . The quotient ring O/P is a finite field. If $q = p^f$ is the number of elements in O/P (p : a prime number, f : a natural number) and β is a uniformizer, then $|\beta| = 1/q$, and the range of values of $|\cdot|$ is $\{q^N : N \in \mathbf{Z}\}$. Further, if S is a complete set of representatives for the residue classes in O/P , every non-zero element $x \in K$ can be written uniquely in the form:

$$x = \beta^{-m}(x_0 + x_1\beta + x_2\beta^2 + \dots),$$

where $m \in \mathbf{Z}$, $x_j \in S$, $x_0 \notin P$. With x written in this form, we have $|x| = q^m$.

3.2. Characters and Fourier transform. We fix a Haar measure μ on K , normalized such that $\mu(O) = 1$. The Fourier transform \mathcal{F} on K is given by

$$(\mathcal{F}f)(\xi) = \int_K f(x)\chi(-x\xi) dx,$$

where χ is a suitably chosen non-trivial character on K , and $dx := d\mu(x)$ refers to the Haar measure just introduced. For our set-up it will be essential to use a *character of rank zero*¹. See [BD15, Subsection 2.1] for a standard way of constructing rank zero characters.

Any Fourier transform based on a rank zero character is an L^2 -isometry with respect to the normalized Haar measure defined above (since $\mathcal{F}\mathbf{1}_O = \mathbf{1}_O$ for any such Fourier transform \mathcal{F} ; $\mathbf{1}$ denotes characteristic function). Thus $\mathcal{F}^{-1} = \mathcal{F}^*$ is given by

$$(\mathcal{F}^{-1}f)(x) = (\mathcal{F}^*f)(x) = \int_K f(y)\chi(xy) dy.$$

¹We remind the reader that the rank of a character χ is defined as the largest integer r such that $\chi|_{B_r} \equiv 1$.

For the rest of this article \mathcal{F} will denote a Fourier transform based on a rank zero character on K .

3.3. Non-Archimedean Schrödinger operator. Our object of study is a version of the Schrödinger operator, defined for \mathbf{Q}_p in the book of Vladimirov, Volovich, Zelenov [VVZ94], and generalized to an arbitrary local field K by Kochubei in [Koc01a]:

$$H = P^\alpha + V,$$

regarded as an operator in $L^2(K)$ ². Here $\alpha > 0$ ³, $P = \mathcal{F}^{-1}Q\mathcal{F}$ where $(Qf)(x) = |x|f(x)$ is the position operator, and \mathcal{F} is the Fourier transform on $L^2(K)$. V (the potential) is multiplication by a *radial* function: $(Vf)(x) = v(x)f(x)$, $v(x) = w(|x|)$ for some function w defined on $[0, \infty)$. We assume v to be non-negative and continuous and that $v(x) \rightarrow \infty$ as $|x| \rightarrow \infty$.

The operator H has been thoroughly analyzed (see [VVZ94] for $K = \mathbf{Q}_p$ and [Koc01a] for general K): It is self-adjoint on the domain $\{f \in L^2(K) : P^\alpha f + Vf \in L^2(K)\}$, has discrete spectrum, and all eigenvalues have finite multiplicity. We will now set up a finite model for this operator.

3.4. Finite model, imbedding, and convergence. Keep the above notation, i.e.: K is a local field, $q = p^f$ is the number of elements in the finite field O/P , β is a uniformizer, and S is a complete set of representatives for O/P . For each integer n set $B_n = \beta^{-n}O =$ ball of radius q^n . Then B_n is an open, additive subgroup of K . For $n > 0$ we set $G_n = B_n/B_{-n}$. Then G_n is a finite group with q^{2n} elements. Since the subgroup B_{-n} will appear quite frequently, we will sometimes denote it by H_n , to emphasize its role as a subgroup. So $H_n = B_{-n} = \beta^n O =$ ball of radius q^{-n} , and $G_n = H_{-n}/H_n$. Each element of G_n has a unique representative of the form $a_{-n}\beta^{-n} + a_{-n+1}\beta^{-n+1} + \cdots + a_{-1}\beta^{-1} + a_0 + a_1\beta + \cdots + a_{n-2}\beta^{n-2} + a_{n-1}\beta^{n-1}$, $a_i \in S$. We denote this set by X_n , and call it *the canonical set of representatives* for G_n ; we also give it the group structure coming from its natural identification with G_n .

Let again μ denote the normalized Haar measure on K (cfr. 3.2). Since H_n is an open subgroup of K , we obtain a Haar measure μ_n on $G_n = H_{-n}/H_n$ by setting $\mu_n(x + H_n) := \mu(x + H_n) = \mu(H_n) = q^{-n}$, for $x + H_n \in G_n$.

So each "point" $x + H_n$ of G_n has mass q^{-n} , and the total mass of G_n is $q^{2n} \cdot q^{-n} = q^n$.

With this choice of Haar measure on G_n the mapping which sends the characteristic function of the point $x + H_n$ in G_n to the characteristic function of the subset $x + H_n$ of K , is an isometric imbedding of $L^2(G_n)$ into $L^2(K)$. The image of $L^2(G_n)$ under this mapping is the subspace $\mathcal{D}_n = \{f \in L^2(K) \mid \text{supp}(f) \subset B_n \text{ and } f \text{ is locally constant of index } \leq q^{-n}\}$ of $L^2(K)$. We regard operators on $L^2(G_n)$ as operators on $L^2(K)$ via this imbedding, setting them equal to 0 on the orthogonal complement of \mathcal{D}_n . Denoting the orthogonal projection on \mathcal{D}_n by D_n , one proves that $\mathcal{F}D_n = D_n\mathcal{F}$. For $f \in \mathcal{D}_n$ and $x \in X_n$ we get

$$\begin{aligned} (\mathcal{F}f)(x) &= \int_K f(y)\chi(-xy)dy = \int_{B_n} f(y)\chi(-xy)dy = \sum_{z \in X_n} \int_{z+H_n} f(y)\chi(-xy)dy \\ &= \sum_{z \in X_n} f(z)\chi(-xz)\mu(H_n) = q^{-n} \sum_{z \in X_n} f(z)\chi(-xz). \end{aligned}$$

²Our operator P is denoted by D in the above cited works.

³For a direct analog of the Laplacian one should set $\alpha = 2$. However, as is customary in the non-Archimedean setting, one works with an arbitrary $\alpha > 0$, since the qualitative behavior of the operator H does not change with $\alpha > 0$.

The last expression coincides with the Fourier transform of f over the finite abelian group G_n . This is because the bicharacter $(x, y) \mapsto \chi(xy)$ of B_n factors through the quotient group $G_n = B_n/B_{-n}$ and defines a non-degenerate bicharacter on G_n , thus implementing the duality of G_n with itself. Denoting the Fourier transform of $L^2(G_n) \simeq \mathcal{D}_n$ by \mathcal{F}_n , we thus have $\mathcal{F}_n = \mathcal{F}|_{\mathcal{D}_n}$.

For the finite versions of the dynamical operators we take their compressions by D_n , i.e., $V_n = D_n V D_n$, $Q_n = D_n Q D_n$, $P_n = D_n P D_n = \mathcal{F}^{-1} Q_n \mathcal{F} = \mathcal{F}_n^{-1} Q_n \mathcal{F}_n$, and set $H_n = P_n^\alpha + V_n$.

For an operator A let P^A denote the projection valued measure associated with A , and for a projection E , let $r(E)$ denote its range. The main convergence theorem in [BD15] was stated as follows:

Theorem 3.1 (Theorem 4.1 in [BD15]).

- (1) If J is a compact subset of $[0, \infty)$ with $J \cap \sigma(H) = \emptyset$, then $J \cap \sigma(H_n) = \emptyset$ for large n .
- (2) If $\lambda \in \sigma(H)$, there exists a sequence (λ_n) with $\lambda_n \in \sigma(H_n)$ such that $\lambda_n \rightarrow \lambda$. Further, if J is a compact neighborhood of an eigenvalue $\lambda \in \sigma(H)$, not containing any other eigenvalues of H , then any sequence λ_n with $\lambda_n \in \sigma(H_n) \cap J$ converges to λ .
- (3) Let again $\lambda \in \sigma(H)$ and let J be a compact neighborhood of λ . Then $\dim P^{H_n}(J) = \dim P^H(J)$ for large n , and for each orthonormal basis $\{e_1, \dots, e_m\}$ for $r(P^H(J))$ there is, for each n , an orthonormal basis $\{e_1^n, \dots, e_m^n\}$ for $r(P^{H_n}(J))$ such that $\lim_{n \rightarrow \infty} e_i^n = e_i$, $i = 1, \dots, m$.

This is the analog of Theorem 4 in [DVV94]; the wording is slightly different, but the content is same.

As was the case in [DVV94] two proofs were given of this theorem: a standard analytic one and a stochastic one. Again, *the stochastic proof gave a stronger convergence result for the eigenfunctions: they were shown to converge uniformly on compacta* (and not just in the L_2 -norm). We comment on both proofs below.

3.5. Comments on the standard analytic proof. There are two main steps in this proof: Establishing the convergence $H_n \rightarrow H$ in the strong resolvent sense, and proving a form of uniform compactness for the resolvents $(I + H_n)^{-1}$. The proofs follow a pattern similar to that of [DVV94], but some arguments can be simplified, partly due to the non-Archimedean nature of K .

3.6. Comments on the stochastic proof. In the stochastic proof one works with the dynamical semigroup generated by the Hamiltonian rather than with the Hamiltonian itself. The aim is to show that $e^{-tH_n} \rightarrow e^{-tH}$ in the trace norm. This will imply the Main Theorem (Theorem 3.1). In addition, it yields the uniform convergence on compacta of the eigenfunctions.

In order to prove convergence in trace norm, one needs to work with the kernel (propagator) of the dynamical semigroup, and to establish Feynman-Kac formulas for the relation between the semigroup and the kernel. The Feynman-Kac formulas in turn require the construction of probability measures on the space of Skorokhod functions over a fixed time interval $[0, t]$. All of this must be done both at the finite and at the infinite level.

With some minor adjustments one uses the same finite models as in the analytic proof. A new feature here is the introduction of stochastics at the finite level.

Stochastics over a local field has been treated by various authors (see, e.g., [Koc01b, Var97, VVZ94]: In analogy with the real case one defines a one-parameter semigroup of probability densities $(p_t)_{t>0}$ as the inverse Fourier transform of what

here corresponds to the Gauss function

$$p_t(x) = (\mathcal{F}^{-1}e^{-t|\cdot|^\alpha})(x) = \int_K e^{-t|\xi|^\alpha} \chi(x\xi) d\xi,$$

and shows that the family $(p_t)_{t>0}$ is indeed a semigroup: $p_{t_1+t_2} = p_{t_1}p_{t_2}$, and that it has all the other required properties:

$$e^{-tP^\alpha} f = p_t * f, \quad p_t(x) > 0 (x \in K), \quad \int_K p_t(x) dx = 1, \quad (*)$$

all relations holding for all $t > 0$. From the densities $(p_t)_{t>0}$ one constructs, for each $a \in K$, a probability measure \mathbf{P}_a on the space of Skorokhod functions⁴ $D([0, \infty) : K)$ such that the following relation holds

$$\int_{D([0, \infty) : K)} f(\omega(t)) d\mathbf{P}_a(\omega) = \int_K f(y) p_t(a - y) dy \quad (3.1)$$

for all f in a suitable class of functions $K \rightarrow \mathbf{C}$. \mathbf{P}_a gives full measure to the paths which start at a . Similarly one constructs, for all $a, b \in K$, $t > 0$, a conditioned probability measure $\mathbf{P}_{a,b,t}$ on $D([0, t] : K)$. This measure gives full measure to the paths which start at a and arrive at b at time t .

At the finite level one mimics the above constructions and defines, for each n , a one-parameter semigroup of probability densities $(p_{t,n})_{t>0}$ by

$$\begin{aligned} p_{t,n}(x) &= (\mathcal{F}_n^{-1}e^{-t|\cdot|^\alpha})(x) = \int_{X_n} e^{-t|\xi|^\alpha} \chi(x\xi) d\mu_n(\xi) \\ &= q^{-n} \sum_{\xi \in X_n} e^{-t|\xi|^\alpha} \chi(x\xi). \end{aligned}$$

Again one shows that the family $(p_{t,n})_{t>0}$ is indeed a semigroup, and that the properties (*) hold, with P_n and $p_{t,n}$ in place of P and p_t .

With the probability densities $(p_{t,n})_{t>0}$ in place, one constructs unconditioned measures \mathbf{P}_a^n and conditioned measures $\mathbf{P}_{a,b,t}^n$ on $D([0, t] : K)$ in the usual way⁵: first on cylinder sets, and then on $D([0, t] : K)$ by verifying the Čentsov condition. Then one shows that the measures \mathbf{P}_a^n and $\mathbf{P}_{a,b,t}^n$ converge weakly to \mathbf{P}_a and $\mathbf{P}_{a,b,t}$, respectively.

Feynman-Kac formulas. Over the local field K :

$$(e^{-tH} f)(x) = \int_K K_t(x, y) f(y) dy, \quad f \in L^2(K), \quad (3.2)$$

where

$$K_t(x, y) = \int_{D[0,t]} e^{-\int_0^t v(\omega(s)) ds} d\mathbf{P}_{x,y,t}(\omega) \cdot p_t(y - x), \quad x, y \in K. \quad (3.3)$$

At the finite level we similarly show:

$$\begin{aligned} (e^{-tH_n} f)(x) &= \int_{X_n} K_t^n(x, y) f(y) d\mu_n(y) \\ &= q^{-n} \sum_{y \in X_n} K_t^n(x, y) f(y), \quad f \in L^2(X_n) \end{aligned} \quad (3.4)$$

⁴ $D([0, \infty) : K)$ is defined as the set of functions $f : [0, \infty) \rightarrow K$ such that f is right continuous on $[0, \infty)$ and $f(s-0)$ exists for all $s > 0$. For a finite interval $[0, t]$ one similarly defines $D([0, t] : K)$ as the set of functions $f : [0, t] \rightarrow K$ such that f is right continuous on $[0, t]$, $f(s-0)$ exists for $s \in (0, t]$, and $f(t) = f(t-)$.

⁵In [BDW17] the unconditioned measures \mathbf{P}_a and \mathbf{P}_a^n were constructed as measures on $D([0, t] : K)$ rather than on $D([0, \infty) : K)$.

where

$$K_t^n(x, y) = \int_{D[0, t]} e^{-\int_0^t v_n(\omega(s)) ds} d\mathbf{P}_{x, y, t}^n(\omega) \cdot p_{t, n}(y - x), \quad x, y \in X_n. \quad (3.5)$$

In order to show convergence in the trace norm, we must first show convergence of the traces, i.e., we must show that

$$\lim_{n \rightarrow \infty} \text{Tr}(e^{-tH_n}) = \text{Tr}(e^{-tH})$$

We have

$$\begin{aligned} \text{Tr}(e^{-tH_n}) &= \int_{X_n} K_t^n(x, x) d\mu_n(x) = q^{-n} \sum_{x \in X_n} K_t^n(x, x) \\ \text{Tr}(e^{-tH}) &= \int_K K_t(x, x) dx, \end{aligned}$$

so it comes down to showing

$$\lim_{n \rightarrow \infty} q^{-n} \sum_{x \in X_n} K_t^n(x, x) = \int_K K_t(x, x) dx.$$

After considerable effort this was achieved in [BDW17]. The proof was patterned on a similar proof in [DVV94]. – With this result in place it was relatively straight forward to prove convergence with respect to the trace norm of the dynamical semigroups. The main result, Theorem 3.1, followed from this, as did the uniform convergence on compacta of the eigenfunctions.

4. MIXED SPECTRUM: ATOMIC POTENTIAL OVER \mathbf{R}^3

The results in this section are taken from the thesis of Erik Makino Bakken [Bak16].

The task is to obtain finite approximations to the operator $H = -\Delta + V$ acting in $L^2(\mathbf{R}^3)$ where $(Vf)(x, y, z) = v(r)f(x, y, z)$, $v(r) = -1/r$, $r = \sqrt{x^2 + y^2 + z^2}$; or, by abuse of notation: $H = -\Delta - 1/r$. This operator is known to be self-adjoint on its natural domain. A notable difference from the situation in the previous sections is that the Coulomb Hamiltonian does not have a compact resolvent, and hence it has a non-empty essential spectrum⁶ – its spectrum $\sigma(H)$ consists of a discrete part $\sigma_{\text{discr}}(H) = \{-\frac{1}{4k^2} : k = 1, 2, 3, \dots\}$ and a continuous part $\sigma_{\text{cont}}(H) = \sigma_{\text{ess}}(H) = [0, \infty)$. Another difference is the singularity at the origin, which makes it difficult to use probabilistic methods, and that approach is not covered in this context.

The author considers a slightly more general situation, and makes the following definition:

Definition 1 (Coulomb-like Operator). Let A be a self-adjoint operator which is bounded below, with discrete spectrum below a constant c , and with $\sigma_{\text{ess}}(A) = \sigma_{\text{cont}}(A) = [c, \infty)$, where $\sigma_{\text{cont}}(A)$ is the continuous spectrum of A . Then we will call A a *Coulomb-like operator*.

Next he defines what he means by convergence of spectra. For this he takes the conclusion of Theorem 3.1, but modifies it to allow for the presence of a continuous spectrum.

⁶In this article the discrete spectrum $\sigma_{\text{discr}}(H)$ of an operator H is defined as the set of isolated eigenvalues of finite multiplicity, and the essential spectrum $\sigma_{\text{ess}}(H)$ is defined as the complement of $\sigma_{\text{discr}}(H)$ in $\sigma(H)$, i.e., $\sigma_{\text{ess}}(H) = \sigma(H) \setminus \sigma_{\text{discr}}(H)$. The continuous spectrum $\sigma_{\text{cont}}(H)$ is generally a subset of $\sigma_{\text{ess}}(H)$.

Definition 2 (Convergence of spectra). Let A be a Coulomb-like operator and let A_n , $n = 1, 2, \dots$ be self-adjoint operators which are bounded below, and let A_n have discrete spectrum. The eigenvalues of A are denoted by $\lambda_1 \leq \lambda_2 \leq \dots$ and are counted with multiplicity. Assume that:

- (1) If J is a compact subset of \mathbb{R} containing no eigenvalues of A , then no eigenvalues of A_n will be in J for sufficiently large n .
- (2) For every $\lambda \in \sigma(A)$ there exists a sequence $\lambda_n \in \sigma(A_n)$ such that $\lambda_n \rightarrow \lambda$. If $J = [a, b]$ is a compact interval with $c < a < b$, then $P_J(A_n)$ converges strongly to $P_J(A)$.
- (3) If J is a compact neighborhood containing the eigenvalue λ_j , and no other eigenvalues of A different from λ_j , then all the eigenvalues of A_n in J converge to λ_j . Furthermore $\|P_J(A_n) - P_J(A)\| \rightarrow 0$ as $n \rightarrow \infty$.

We will then say that the spectrum of A_n converges to the spectrum of A , and we will denote it by

$$\sigma(A_n) \rightarrow \sigma(A). \quad (4.1)$$

The finite model is the same as in Section 2 (with $n = 3$), with a specific choice of boundary conditions for the Laplacian.

4.1. Approximation in a cube. The author first discusses convergence of spectra within a fixed open cube $T_b = \{(x_1, x_2, x_3) \in \mathbb{R}^3 : |x_i| < b, i = 1, 2, 3\}$. The idea is to show that, in a finite box, the Hamiltonian has compact resolvent and hence discrete spectrum. This makes available much of the proof techniques used in [DVV94].

When restricted to the cube, the operators are given the index b : $H_b = -\Delta_b + V_b$; here Δ_b is the Laplacian restricted to the cube, whereas the function v_b , which defines V_b , is modified to handle the singularity at the origin:

$$v_b(r) = \begin{cases} -\frac{1}{r} & \text{if } r > 1/b \\ -b & \text{if } r \leq 1/b. \end{cases} \quad (4.2)$$

The author then shows that H_b does, indeed, have compact resolvent and hence discrete spectrum.

For the finite grid inside the cube, the author sets $\epsilon = 2b/(n+1)$ (the grid spacing) and indexes the operators on the grid with the two parameters b, n : $H_{b,n} = -\Delta_{b,n} + V_{b,n}$. With the above result in hand (compact resolvent etc.) he is able to show that $\lim_{n \rightarrow \infty} \sigma(H_{b,n}) = \sigma(H_b)$ in the sense of Definition 2, or – since H_b has discrete spectrum – in the sense of Theorem 2.1 or Theorem 3.1.

4.2. Approximation in all of \mathbb{R}^3 . Finally the author must take the limit as $b \rightarrow \infty$, at the same time as the grid spacing goes to zero, i.e., $b/n \rightarrow 0$. This requires a certain dependence of n on b , call it $n(b)$. A short version of his final theorem can be stated as follows:

Theorem 4.1. *Let as before H be the Coulomb Hamiltonian, and let $H_{n,b}$ be the finite Hamiltonian as above. There exists an assignment $b \rightarrow n(b)$ such that $\lim_{b \rightarrow \infty} \sigma(H_{b,n(b)}) = \sigma(H)$ in the sense of Definition 2.*

This is an existence theorem and doesn't lend itself readily to computations, as it doesn't tell us how to choose the function $b \rightarrow n(b)$. It does, however, show that the Coulomb Hamiltonian can be obtained as a limit of *some* sequence of finite Hamiltonians of the type described above, a result which is of independent interest.

One can make educated guesses as to the growth of the function $b \rightarrow n(b)$. In the Appendix we present a computer run with $n(b) \sim b^2$. As can be seen there, the numerically computed values show remarkable agreement with the exact theoretical values.

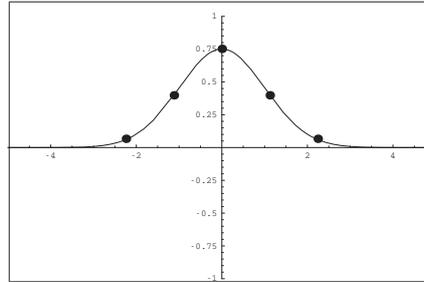
APPENDIX A. NUMERICAL RESULTS

A.1. Numerics for the harmonic oscillator over \mathbf{R} .

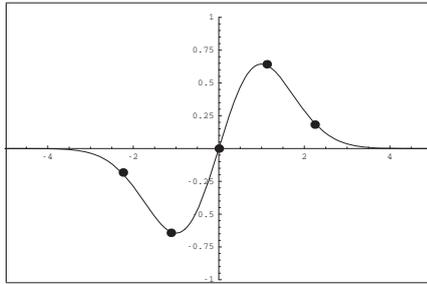
A1a The three groups of figures below show eigenvalues and eigenfunctions for the harmonic oscillator over the \mathbf{R} with 5, 21 and 81 points in the grid, respectively.

Eigenvalues for H_5

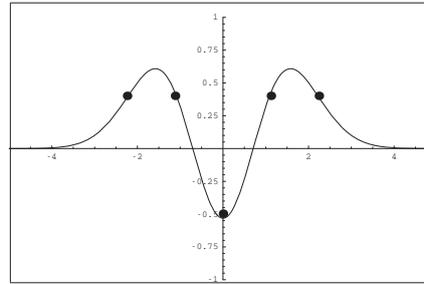
0.4969786369997017
 1.538153655416401
 2.273277799898967
 3.512928870280916
 4.745031651763187



Eigenfunction no. 0
 for H_5 (dotted) and H (smooth).



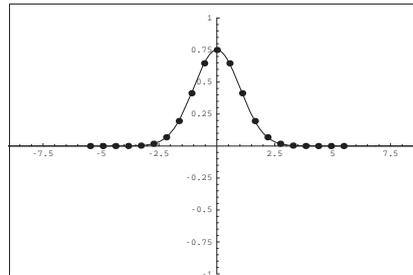
Eigenfunction no. 1
 for H_5 (dotted) and H (smooth).



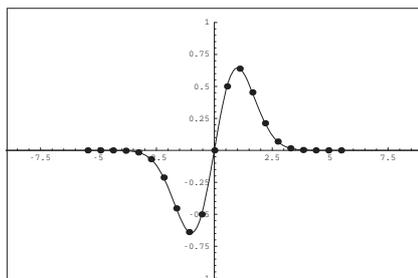
Eigenfunction no. 2
 for H_5 (dotted) and H (smooth).

Eigenvalues for H_{21}

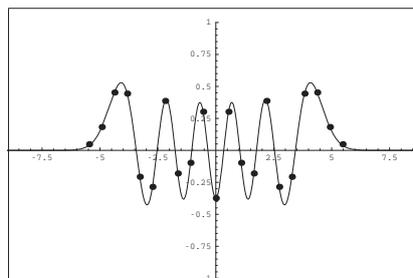
0.4999999999999396
 1.50000000000396
 2.499999999873056
 3.50000002436515
 4.499999963136251
 5.500000389175935
 6.499996311530578
 7.500024950572093
 8.499832644686019
 9.500769902078664
 10.49608851334482



Eigenfunction no. 0
 for H_{21} (dotted) and H (smooth).



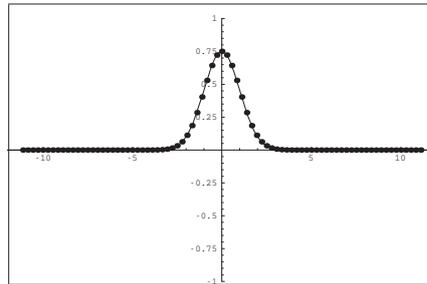
Eigenfunction no. 1
 for H_{21} (dotted) and H (smooth).



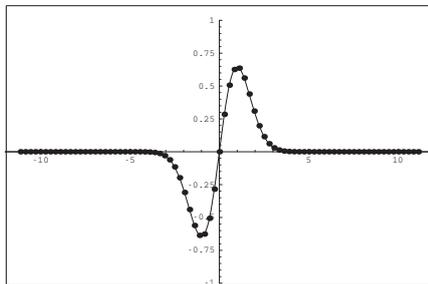
Eigenfunction no. 10
 for H_{21} (dotted) and H (smooth).

Eigenvalues for H_{S1}

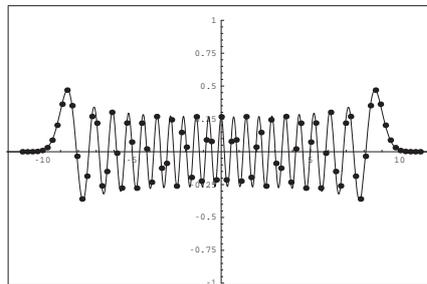
0.500000000000002
 1.500000000000014
 2.500000000000016
 3.499999999999992
 4.499999999999959
 5.5
 6.500000000000021
 7.500000000000014
 8.499999999999976
 9.500000000000012
 10.5



Eigenfunction no. 0
 for H_{S1} (dotted) and H (smooth).



Eigenfunction no. 1
 for H_{S1} (dotted) and H (smooth).



Eigenfunction no. 40
 for H_{S1} (dotted) and H (smooth).

A1b The two tables below show a comparison between the Schwinger method and the standard finite difference method for the finite models of the real harmonic oscillator. As can be seen, the Schwinger method gives far better numerical results.

N=81, 7 decimals

Exact	Schwinger	Finite diff.
1/2	0.5000000	0.4975640
3/2	1.5000000	1.4877712
5/2	2.5000000	2.4680608
7/2	3.5000000	3.4382768
9/2	4.5000000	4.3982546
11/2	5.5000000	5.3478205
13/2	6.5000000	6.2867905
15/2	7.5000000	7.2149698
17/2	8.5000000	8.1321509
19/2	9.5000000	9.0381131
21/2	10.5000000	9.9326202

N=241, 7 decimals

Exact	Schwinger	Finite diff.
1/2	0.5000000	0.4991839
3/2	1.5000000	1.4959143
5/2	2.5000000	2.4893615
7/2	3.5000000	3.4795090
9/2	4.5000000	4.4663402
11/2	5.5000000	5.4498380
13/2	6.5000000	6.4299851
15/2	7.5000000	7.4067638
17/2	8.5000000	8.3801562
19/2	9.5000000	9.3501440
21/2	10.5000000	10.3167088

A.2. Numerics for the harmonic oscillator over $\mathbf{Q}_3[\sqrt{3}]$.

A2a Harmonic oscillator $H = \frac{1}{2}(P^2 + Q^2)$ over $\mathbf{Q}_3[\sqrt{3}]$: Numerically computed eigenvalues.

A shell function is a function which is supported on a single shell (sphere) about the origin. A radial function is one which is constant on each shell.

Theoretical eigenvalue	Numerical eigenvalue	Theoretical multiplicity	Numerical multiplicity	Type of eigenfunction	Comment
$0 < \lambda_0 < 9/13$ ≈ 0.6923	0.6684	1	1	radial	
?	4.6922	?	1	radial	
?	4.7158	?	1	radial	
5	5.0000	2	2	shell function	$2 = 1 + 1$: Coming from two different shells.
9	9.0000	4	4	shell function	All supported on the same shell.
?	40.5213	?	2	radial	
$40 + 5/9 =$ $40.5555\dots$	40.5555	2	2	shell function	$2 = 1 + 1$: Coming from two different shells.
41	41.0000	8	8	shell function	$8 = 4 + 4$: Coming from two different shells.
45	45.0000	24	24	shell function	$24 =$ $12 + 12$: Coming from two different shells.

A.3. Numerics for the Coulomb Hamiltonian in \mathbf{R}^3 . The table shows numerically computed eigenvalues of a scaled Coulomb Hamiltonian (i.e., eigenvalues are of the form $-\frac{1}{k^2}$ rather than $-\frac{1}{4k^2}$). The computation is done with $n = 350$ (i.e., 350^3 points in the grid) and spacing $\varepsilon = (2\pi/n)^{1/2}$.

Exact values	Numerical values
-1	-0.9814558
-1/4	-0.2505890, -0.2505890, -0.2505890, -0.2483674
-1/9	-0.11136023, -0.11136023, -0.11136023, -0.11121653, -0.11121653, -0.1111883, -0.1111883, -0.1111883, -0.1106982
-1/16	-0.06260630, -0.06260630, -0.06260630, -0.06254948, -0.06254948, -0.06254293, -0.06254293, -0.06254293, -0.06252377, -0.06252377, -0.06252377, -0.06252227, -0.06252227, -0.06252227, -0.06251815, -0.06231906

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