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Autor: Knill, Oliver
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A remark on quantum dynamics

By Oliver Knill

Department of Mathematics,
University of Arizona, Tucson, AZ, 85721, USA,
e-mail: knillmath.arizona.edu

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Abstract

Some computations in classical quantum dynamics can be simplified by substituting the Schrödinger Hamiltonian with a different operator. The time evolution can then be obtained by iterating a map. This allows efficiently to determine the Fourier coefficients of the spectral measures of the new Hamiltonian. Many properties of the quantum evolution are not affected by the deformation of the Hamiltonian because the spectral measures are only distorted. For example, a numerical computations of the Wiener averages allows to test numerically for the existence of bound states. We illustrate the time discretisation for a tight binding model of an electron in a constant or random magnetic field in the plane. As a theoretical illustration, we relate the return probability for the quantum evolution on a graph to the return probability of the corresponding random walk.

1 Introduction

For numerical simulations in quantum mechanics it is important that the orbits $\psi(t) = \exp(itL)\psi$ of the quantum evolution can be determined efficiently. Even for a bounded operator L, the computation of $\exp(itL)\psi$ can become tremendous; in higher dimensions it is a task for super computers (e.g. [23]).

Many properties of the orbit $\psi(t)$ are determined by the spectral measures μ_ψ which are probability measures on the real line. Dynamical properties of the system depend on the nature of the spectral measure because the Fourier transform of μ_ψ is $\hat{\mu}_\psi(t) = (\psi, \psi(t))$. For example, a Hamiltonian L with absolutely continuous spectrum leads by the Rieman-Lebesgue lemma to the transient behavior $(\psi, \psi(t)) \to 0$. On the other hand, if an operator L has purely discrete spectrum, then $(\psi, \psi(t))$ is almost periodic a fact which is responsible for recurrent behavior of the dynamics.

In this note, we use the fact that it is often irrelevant, whether we evolve with the Hamiltonian L or if we use a deformed Hamiltonian $f(L)$, where f is an invertible smooth real function. The reason is that the spectral measures of $f(L)$ are only distorted versions of the spectral measures of L. It is therefore natural, to look for a function f such that the discrete time step $\exp(if(L))$ can be easily computed. Properties of the spectrum, which are unchanged by a replacement $L \rightsquigarrow f(L)$ can now be determined faster through numerical experiments because iterating a map is more simple than integrating a differential equation.

If $\tilde{L} = \arccos(aL)$ where L has been rescaled such that aL has norm smaller or equal to 1, the time evolution can be computed by iterating the map $A : (\psi, \phi) \mapsto (2aL\psi - \phi, \psi)$ on $H \oplus H$. This is the time one map for the unitary evolution of $\tilde{L}$. This allows an efficient determination of the Fourier coefficients $\hat{\mu}_n = (\psi, \psi(n))$ with $A^n(\psi, 0) = (\psi(n), \phi(n))$ of measures μ_ψ on the circle, which determine the spectral measures ν_ψ of L. Some properties of the quantum evolution are not affected by the change $L \mapsto \tilde{L}$ because the spectral measures $\tilde{\nu}$ of $\tilde{L}$ and the spectral measure ν of L are related by $\tilde{\nu}(I) = \nu(\cos(I))$ for every interval I.

One possibility to test for discrete spectrum of an operator is to determine numerically the Wiener averages $\lim_{n\to\infty} n^{-1} \sum_{k=1}^{n} |\hat{\mu}_k|^2 = \sum_x |\mu\{x\}|^2$. We illustrate this method for a tight binding model of an electron in a constant or random magnetic field in the plane. For random magnetic fields, where the existence of point spectrum is not known, we made numerical experiments on a grid of size up to 1000×1000.

We also illustrate the theoretical usefulness of the discrete time evolution by providing a relation between quantum mechanical return probabilities of the generator for a random walk on a graph and the return probability of the classical random walk on a graph: continuity properties of spectral measures with respect to the α-dimensional Hausdorff measures are related to power-law decays of averaged return probabilities of the random walk.

2 A unitary discretisation

Let L be a bounded selfadjoint operator on a separable Hilbert space H. After a rescaling $L \mapsto aL$, which corresponds to a change of time in the evolution, we can assume that $||L|| \leq 1$. Assume $\tilde{L}$ solves $\cos(\tilde{L}) = L$. The unitary operators $U_\pm^n = \exp(\pm in\tilde{L})) = \cos(in \arccos(L)) \pm i \sin(in \arccos(L)) = T_n(L) \pm iR_n(L)$ are independent of the choice of $\tilde{L}$. Both $U_\pm = L \pm i\sqrt{1-L^2}$ solve $U + U^* = 2L$ and $U_\pm$ has its spectrum in $\{\pm\ \mathrm{Im}(z) > 0\}$. Here $T_n(x) = \cos(n \arccos(x))$ is the *n'th* Chebychev polynomial of the first kind and $R_n(x) = \sin(n \arccos(x))$ is the n'th Chebychev function of the second kind.

Proposition 2.1 *If $\psi(t) = \exp(it\tilde{L})\psi(0)$, then $\psi(t)$ evaluated at integer times satisfies the recursion $\psi(n+1) + \psi(n-1) = 2L\psi(n)$. Solutions of this recursion are given by $\psi_\pm(n) = U_\pm^n\psi$. In particular, $\psi(n) = (\psi_+(n) + \psi_-(n))/2$ is a solution, which is real if $\psi(0)$ is real.*

Proof. $U_\pm + U_\pm^* = 2L$ implies that $\psi_\pm(n) = U_\pm^n\psi$ as well as the linear combination $\psi(n)$ satisfy this recursion. □

The discrete time evolution is obtained by iterating the map

$$A : (\psi, \phi) \mapsto (2L\psi - \phi, \psi) \tag{2.1}$$

on $H \oplus H$. The unitary nature of the evolution is also evident because

$$A = \begin{pmatrix} 2L & -1 \\ 1 & 0 \end{pmatrix}, \quad B = \begin{pmatrix} \exp(i \arccos(L)) & 0 \\ 0 & \exp(-i \arccos(L)) \end{pmatrix}$$

on $H \oplus H$ are conjugated by $A = C^{-1}BC$ using $C = \begin{pmatrix} L - i\sqrt{1-L^2} & L + i\sqrt{1-L^2} \\ 1 & 1 \end{pmatrix}$.

3 The Fourier coefficients of the spectral measures

For $\psi \in H$, the functional $f \mapsto (\psi, f(L)\psi)$ defines by Riesz representation theorem a measure ν_ψ on $[-1, 1]$, which is the spectral measure of ψ. On the circle $\mathbf{T}$, we are interested in the spectral measures $\mu_{\psi,\pm}$

with respect to the unitary operators $U_\pm$ which are also determined by their Fourier coefficients $(\hat{\mu}_{\psi,\pm})_n = (\psi, U_\pm^n \psi)$. Let $\tilde{\nu}_\psi$ be the spectral measure of ψ with respect to $\tilde{L}$. These measures are related as follows:

Proposition 3.1 *For every Borel set Y on $[0,\pi]$ one has $\tilde{\nu}_\psi(Y) = \nu_\psi(\cos(Y))$. The measure $\mu_\psi = (\mu_{\psi,+} + \mu_{\psi,-})/2$ satisfies $\nu_\psi((Z+\overline{Z})/2) = \mu_\psi(Z)$ for every Borel set Z on the circle.*

Proof. The first statement follows from the relation $\int \exp(itx)\, d\nu(\cos(x)) = \int \exp(it \arccos(x))\, d\nu(x) = (\psi, \exp(i \arccos(L))\psi) = (\psi, \exp(it\tilde{L})\psi) = \int \exp(itx)\, d\tilde{\nu}(x)$. The formula $U_\pm + U_\pm^* = 2L$ implies the second relation. □

Remarks.
1) The measure μ_ψ on $\mathbf{T}$ is a spectral measure of $\psi \times \psi$ of the unitary operator $U = U_+ \oplus U_-$ on $H \oplus H$ which gives a the simultaneous evolution of ψ_+ and ψ_- on two copies of the Hilbert space H.
2) The study of orthogonal polynomials on $[-1,1]$ by lifting them onto the circle goes back to Szegö [29]. In [7], it was suggested to replace ordinary moments $\int x^n\, d\mu$ by other moments $\int p_n(x)\, d\mu$ in order to get information on the spectral measures of operators. However, the case of Chebychev polynomials treated here has been left out in [7]. We should note that Chebychev polynomials are also useful in similar contexts like polynomial expansions of the Green functions (see [21]).

Proposition 3.2 *The Fourier coefficients of the spectral measure $\mu = \mu_\psi = (\mu_{\psi,+} + \mu_{\psi,-})/2$ satisfy*

$$(\hat{\mu}_\psi)_n = (\psi, T_n(L)\psi) = (\psi, \psi(n)) .$$

Proof. We have $(\hat{\mu}_{\psi,\pm})_n = \int_{\mathbf{T}} e^{-int}\, d\mu_{\pm,\psi}(t) = (\psi, U_\pm^n \psi)$ so that

$$(\hat{\mu}_\psi)_n = (\hat{\mu}_{\psi,+})_n + (\hat{\mu}_{\psi,-})_n = (\psi, (U_+^n + U_-^n)/2\psi) = (\psi, T_n(L)\psi) .$$

This, together with the definition $(U_+^n + U_-^n)\psi/2 = (\psi_+(n) + \psi_-(n))/2 = \psi(n)$ implies the claim. □

4 Spectral properties and the dynamics

We review in this section some spectral properties which can be deduced from Fourier coefficients $(\psi, \psi(n))$ of spectral measures.

The discrete spectrum. Wiener's theorem in Fourier theory

$$\lim_{n\to\infty} n^{-1} \sum_{k=1}^{n} |(\psi, U^k \psi)|^2 = \lim_{n\to\infty} n^{-1} \sum_{k=1}^{n} |\hat{\mu}_k|^2 = \sum_{x \in \mathbf{T}} \mu(\{x\})^2$$

allows to determine, whether there is some discrete part in the spectral measure μ_ψ and so some eigenvalues of L. This tool for detecting point spectrum is used in quantum dynamics (see [1]). If the potential takes finitely many (rational) values, then $n^{-1} \sum_{k=1}^n |\hat{\mu}_k|^2$ is a (rational) number which can be computed exactly. Evolution (2.1) allows so to treat the evolution of any bounded discrete Schrödinger operators in one dimension with the same efficiency as kicked quantum oscillators or kicked Harper models.

The L^2-absolutely continuous spectrum. If there exists a constant C, such that $\sum_{k=1}^n |(\psi, U^k\psi)|^2 \leq C$ then $\mu_\psi \in L^2$, because of Plancherel's theorem $\sum_{k=1}^n |(\psi, U^k\psi)|^2 \to \int |f_\psi|^2\, d\theta$ with $\mu_\psi(\theta) = f d\theta$. It is more difficult to detect other absolutely continuous spectrum. While $\hat{\mu}_n$ goes to zero by the Riemann-Lebesgue lemma, if μ is absolutely continuous, the decay can be arbitary slow and decay is also possible if μ is singular continuous. The L^2-absolutely continuous spectrum is important because by a result of Kato, the closure of all vectors ψ with L^2-absolutely continuous spectral measures μ_ψ is the absolutely continuous subspace.

Singular continuous spectrum. If $(\psi, U^n\psi)$ does not converge to zero, then by the Riemann-Lebesgue theorem, μ_ψ must have some singular spectrum. If also $n^{-1}\sum_{k=1}^n |(\psi, U^k\psi)|^2$ converges to zero, then L has purely singular continuous spectrum, a property, which is generic in many situations (see [25, 27]). However, if L has purely singular continuous spectrum, it is still possible that $(\psi, U^n\psi) \to 0$. The question, whether $(\psi, U^n\psi)$ converges to zero or not can be subtle and there are both singular continuous measures for which $(\psi, U^n\psi)$ does or does not converge to zero. Singular continuous spectrum occurs often in solid state physics. The dynamics of U on the singular continuous subspace is the least understood. It follows from Wiener's theorem and Birkhoff's ergodic theorem that the topological entropy of an unitary operator acting on the weakly compact unit ball is zero [16].

Weak continuity properties. A discrete version of a result of Stricharz [28] tells that if there exists a constant C and a function $h \in C(\mathbf{R})$ with $h(0) = 0$ such that $\mu([a,b]) \leq Ch(|b-a|)$ for all intervals $[a,b]$ with length < 1 on the circle $\mathbf{R}/(2\pi\mathbf{Z})$ (here identified with $[0, 2\pi)$), then

$$n^{-1}\sum_{k=1}^{n} |(\psi, U^n\psi)|^2 \leq C_1 C h(n^{-1}) \tag{4.1}$$

for all n, where $C_1 < 10$ is a constant independent of anything. By a converse of Last [19], if Equation (4.1) is satisfied, then $\mu([a,b]) \leq C\sqrt{h(|b-a|)}$ for all intervals $[a,b]$. In this sense, Hölder continuity properties of the distribution function $x \mapsto \int_a^x d\mu_\psi(t)\, dt$ can be detected by computing $(\psi, U^n\psi)$. For recent developments in the quantum dynamics of operators with singular continuous spectrum see [9, 5, 10, 19].

Hausdorff dimension. The α-energy of a spectral measure μ on $\mathbf{T}$ is $I_\alpha(\mu) = \int_{\mathbf{T}^2} \phi_\alpha(\sin(\frac{x-y}{2}))\, d\mu(x)\, d\mu(y$ with $\phi_\alpha(x) = x^{-\alpha}, \phi_0(x) = -\log|x|$. A measure $\mu = \mu_f$ has finite α-energy, if and only if $\sum_{k=1}^\infty k^{\alpha-1}|\hat{\mu}_k|^2 < \infty$ ([13]). The Hausdorff dimension of μ, is the minimum of all Hausdorff dimensions of Borel sets S satisfying $\mu(S) = 1$. It is bigger or equal to α if μ has finite α-energy (see Theorem 4.13 in [6]). By finding out, where the energy blows up, a lower bound on the Hausdorff dimension of μ can be established and so a lower bound on the Hausdorff dimension of the support of μ can be obtained.

5 Quantum dynamics versus random walks

Assume L is the generator of a random walk on a graph (V, E) where V is the set of vertices and E is the set of edges. The hopping probabilities $p_{(v,w)} = p_{(w,v)}$ to the vertices so that $\sum_{w,(v,w)\in V} p_{(v,w)} = 1$ define the random walk. For example, if every edge has d neighbours and $p_{w,v} = 1/d$ for every vertex (w,v), we get a symmetric random walk on a regular graph. The operator $L\psi(v) = \sum_{(w,v)\in V} p_{w,v}\psi(w)$ is selfadjoint and has norm 1. Let $\psi_v \in l^2(V)$ be a wave which is localized initially at a vertex v. The quantum evolution $T_n(L)\psi_v = \mathrm{Re}(\exp(in\arccos(L)))\psi_v$ should be compared with the random walk $L^n\psi_v$: while $\rho_n = (\psi_v, L^n\psi_v)$ is the probability that the walker starting at the vertex v returns to v in n steps, $\hat{\mu}_n^2 = (\psi_v, T_n(L)\psi_v)^2$ is the probability that the wave ψ_v returns back after n steps of the quantum evolution. Opposite to the irreversible random walk, the discrete time quantum evolution is invertible in the sense that the pair $\psi(n), \psi(n+1)$ determines $\psi(0)$. The Fourier coefficients $\hat{\mu}_n = (\psi, \psi(n))$ of μ are easy to compute and determine the measures $\nu = 1/2(\mu + \overline{\mu})$ of ψ with respect to L. In many examples of regular infinite graphs, one does not know the spectral type. Aperiodic graphs defined by aperiodic tilings of $\mathbf{R}^d$ (see [18, 17]) are examples, where the spectral type is unknown. The spectrum of a graph can be be pure point like in the case of a finite graph or certain self-similar graphs, it can be absolutely continuous like for $\mathbf{Z}^d$ or for Cayley graphs of infinite Abelian discrete groups, it can also be singular continuous as has been pointed out recently in [26].

In order to relate the return probability of the random walk with the Fourier coefficients, we consider a one parameter family of operators $L(\theta) = L\cos(\theta)$. Denote by $\hat{\mu}_n(\theta) = T_n(L(\theta))_{00}$ the Fourier coefficients of the spectral measure on the circle with respect to the operator $L(\theta)$.

Proposition 5.1 *The probability ρ_n that the random walk starting at the vertex v returns to v in n steps is related to the quantum mechanical return probability $\hat{\mu}_n^2(\theta)$ of the discrete unitary quantum evolution of $L(\theta)$ by*

$$(4\pi)^{-1} \int_{\mathbf{T}} \hat{\mu}_n(\theta)^2 \, d\theta \geq \rho_n^2 .$$

Proof. With $z = \exp(i\theta)$, we have $L(\theta) = L(z + z^{-1})/2$. The function $f_n(z) = z^{n-1}\hat{\mu}_n(z)$ is a sum of an analytic part and L_{00}^n/z so that by Cauchy's formula $\int_{|z|=1} f_n(z)\, dz = f(0) = L_{00}^n = \rho_n$. Because ρ_n is real, we get

$$(2\pi)^{-1} \int_{\mathbf{T}} \cos(2n\theta)\hat{\mu}_n(\theta) \, d\theta = \rho_n .$$

With Hölder inequality, we have

$$\rho_n = (2\pi)^{-1} \int_{\mathbf{T}} \cos(2n\theta)\hat{\mu}_n(\theta) \, d\theta \leq ((4\pi)^{-1} \int_{\mathbf{T}} \hat{\mu}_n^2(\theta) \, d\theta)^{1/2} .$$

□

Corollary 5.2 *If the spectral measure $\mu_v(\theta)$ satisfies $\mu_v(\theta)[a,b] \leq C(\theta)h(b-a)$ for all intervals strictly contained in the circle $\mathbf{T}$ and all $\theta \neq \pi/2$, and if $\int C(\theta)\, d\theta < \infty$, then the random walk has the return property $n^{-1}\sum_{k=1}^n \rho_k^2 \leq C_1 \int C(\theta)\, d\theta h(n^{-1})$, where C_1 is a constant not depending on anything.*

Proof. Consider the relation

$$\int_{\mathbf{T}} n^{-1} \sum_{k=1}^n (4\pi)^{-1}\hat{\mu}_k^2(\theta) \, d\theta \geq n^{-1} \sum_{k=1}^n \rho_k^2$$

Applying Strichartz theorem described in the last section, we get from $\mu_v(\theta)[a,b) \leq C(\theta)h(b-a)$ that the left hand side is $\leq C_1 \int_{\mathbf{T}} C(\theta)\, d\theta h(n^{-1})$ with some universal constant C_1. (In the case $h(x) = x$, $C(\theta)$ does not depend on θ. It follows that if a graph has a uniform return probability like on a finite graph, then by Wiener's theorem, there is some point spectrum implying quantum mechanical recurrence). □

A measure μ_v is called uniformly α-continuous if $\mu_v[a,b) \leq C(b-a)^\alpha$ for all intervals $[a,b)$.

Corollary 5.3 *If the spectral measure μ_v is uniformly α-continuous, then the return probabilities of the random walk to the vertex v satisfy $n^{-1}\sum_{k=1}^n \rho_k^2 \leq n^{-\beta}$ for all $\beta < \alpha$ and large enough n.*

Proof. Because $C(\theta) \leq \cos(\theta)^{-1}C(0)$ it follows that $\int_{\mathbf{T}} C(0)\cos(\theta)^{-\epsilon} d\theta < \infty$ for all $\epsilon > 0$. Apply Corollary 5.2 gives $n^{-1}\sum_{k=1}^n \rho_k^2 \leq C_1 \int_{\mathbf{T}} C(\theta) n^{-\alpha} \leq n^{-\beta}$ for large n. □

6 Numerical experiments

We illustrate the discrete time evolution (2.1) in two numerical experiments.

(i) The first numerical experiment deals with an electron in the plane under a constant magnetic field B reduced by a Landau gauge to a one-dimensional situation, where one considers the one-dimensional Schrödinger operator L on $l^2(\mathbf{Z})$ of the form $Lu(n) = \Delta u(n) + V(n)u(n)$ and take an initial condition which is a localized wave $\psi(0) = (\cdots, 0, 0, 0, 1, 0, 0, 0, \cdots)$ at the origin $k = 0$. We use Wiener's theorem to get numerically information about the discrete part of the spectral measure. For this illustration, we take the almost Mathieu (or Harper) operator $V_n = \lambda \cdot \cos(\theta + \alpha n)$, where much about the spectrum is known (see [24, 20, 11] for reviews). Note that most of the known results hold only for almost all or generic θ and under some assumptions on the magnetic flux α.

We did a numerical determination of $S_n(\lambda) = n^{-1} \sum_{k=1}^{n} |\hat{\mu}_k|^2$ using (2.1), up to $n = 40'000$ as a function of $\lambda \in [0, 4]$ in the almost Mathieu operator with $\theta = \sqrt{3}, \alpha = \sqrt{7}$. μ is the spectral measure on the circle belonging to the vector $\psi = \delta_0$ localized at the origin in $\mathbf{Z}$. The value of $\hat{\mu}_n = (\psi, U^n \psi)$ was computed using evolution (2.1) with initial condition $(\psi, 0)$ on the grid $[-n/2, n/2]$ so that the boundary effects the value $\hat{\mu}_n$ only after n steps: $\psi(n)$ has support in $[-n, n]$ and the boundary begins to affect ψ after $n/2$ time steps and so to influence $\hat{\mu}_n$ after n steps. The numerical experiment is in agreement with the now established fact that there is no point spectrum for $\lambda \leq 2$ for almost all α (for $\lambda = 2$ see [8]) and some point spectrum for $\lambda > 2$ [12]. Longer runs, $(S_{10000}(2) = 0.004858, S_{20000}(2) = 0.001900, S_{40000}(2) = 0.001068)$ indicated that indeed $S_n(2) \to 0$ for $n \to \infty$.

(ii) In a second numerical experiment, we take a two dimensional operator L which is the Hamiltonian for an electron in the discrete plane, where the magnetic field B is randomly taking values in $U(1)$ (see [15] for some theoretical results or [3, 2] for other numerical experiments on this model). If the distribution of $B(n), n \in \mathbf{Z}^2$ is a Haar measure of $U(1)$, then this field can be generated with a vector potential $A_i(n) = e^{i\theta(n)}$ with independent random variables $\theta(n)$ having the uniform distribution in $[0, 2\pi]$. There is no free parameter. The ergodic operator, which we consider, is

$$L\psi(n) = A_1(n)\psi(n + e_1) + \overline{A_1(n - e_1)}\psi(n - e_1) + A_2(n)\psi(n + e_2) + \overline{A_2(n - e_2)}\psi(n - e_2)$$

and the open question is what is the spectral type of L.

While one knows the moments of the density of states of L (the n-th moment of the density of states is the number of closed paths in $\mathbf{Z}^2$ of length n starting at 0 which give zero winding number to all plaquettes [16]), nothing about the spectral type of L seems to be known. For the two dimensional experiment, we experimented on a 1000×1000 lattice, were we can compute the first 1000 Fourier coefficients of the spectral measure exactly. Our experiments indicate no eigenvalues. If eigenvalues exist, they would have to be extremely uniformly distributed because $\lim_{n\to\infty} S_n = \sum_x |\mu\{x\}|^2$ must be small. The measurements done on a usual workstation indicate that S_n goes to zero monotonically: $S_{200} = 0.00352372, S_{400} = 0.00201089, S_{600} = 0.00148669, S_{800} = 0.00121992, S_{1000} = 0.00106374$. Longer runs with better computers on larger lattices are needed to confirm this picture.

Remark. We made also numerical experiments with a Aharonov-Bohm problem on the lattice. This is the situation when the magnetic field B is different from 1 only at one plaquette $n = (0, 0)$. The vector potential A in this situation can not be chosen differently from 1 in a compact set. However, in a suitable gauge, the operator L is a compact perturbation of the free operator by a result of Mandelstham-Jitomirskaja [22] see [16] for an other proof of this fact). As expected, there was no indication of some discrete spectrum. The numerical experiments suggest that $\sum_k |\hat{\mu}_k|^2$ is bounded which would mean that the spectral measures are in L^2.

7 Relations with other numerical methods

The usual Schrödinger evolution $\exp(itL)$ needs a numerical integration like $\exp(itL)\psi \sim (1+\frac{it}{n}L)^n\psi$, where n is so large that $t^n/n!$ is smaller than the desired accuracy ϵ. Any such truncation produces high-frequency noise after a relatively small number of time steps. An other method used in quantum dynamics is to diagonalize a finite dimensional approximation L_N of L and to evolve its eigenfunctions (see for example [14]). It is quantitatively not clear, how well a finite dimensional Galerkin cut-off respects the actual dynamics. Moreover, in dimension d, the number of grid points N has to be so small that an eigensystem of a N^d matrix can be found.

While numerical approximations of $\exp(itL)$ are not unitary, the evolution (2.1) is conjugated to a unitary evolution. Other discrete unitary time evolutions have been considered in [4]. The problem to preserve unitarity is similar to numerical integration problems for ODE's, where for example symplecticity should be preserved during the discretisation of a Hamiltonian system.

If $\psi(0)$ has compact support, then $\psi(n)$ has this property too. This leads to a finite propagation speed as in a relativistic set-up. This fact has computational advantages. For example, we know exactly, after which time, boundary effects begin to influence the value of a wave at some point.

The discrete evolution preserves the (not necessarily closed) algebraic field in which L is defined. For example, if L is an operator defined over the rationals $\mathbf{Q}$ and if the coordinates of $\psi(0)$ are rational, then $\psi(t)$ is rational and $\hat{\mu}_n \in \mathbf{Q}$ can be determined exactly.

The evolution (2.1) can be defined on all bounded sequences $l^\infty(\mathbf{Z}^d)$ and not only on $l^2(\mathbf{Z}^d)$. For example, the evolution leaves almost periodic configurations invariant, elements $x \in l^\infty(\mathbf{Z}^d)$, for which the closure of all translated sequences $(T^n x)(k) = x(k+n)$ is compact in the uniform topology $d(x,y) = \max_{k\in\mathbf{Z}^d}|x(k)-y(k)|)$. This is useful, because solutions of (2.1) define generalized eigenfunctions $K\psi = 0$ of an operator K defined on space-time.

The unitary operator $V = -iU$ solves $i(V-V^*) = 2L$ which is a discretisation of the Schrödinger equation $i\dot{U} = 2L$. Since $V^4 = U^4$, the evolutions U and V are essentially the same. The discrete evolution $V^n\psi$ is a second order approximation to $\exp(it2L)\psi$ in the sense that $\exp(i\arcsin(2\epsilon L)) = 1-2i\epsilon L - 2\epsilon^2L^2 - 2\epsilon^4L^4\dots$ and $u \mapsto \exp(2i\epsilon L) = 1 - 2i\epsilon L - 2\epsilon^2L^2 + \frac{4}{3}i\epsilon^3L^3 + \frac{2}{3}\epsilon^4L^4\dots$ agree up to second order. This second order approximation is more efficient than the second order but computationally more expensive Cayley method $(\epsilon L - i)(\epsilon L + i)^{-1} = \exp(2i\arctan(\epsilon L)) = 1 - 2i\epsilon L - 2\epsilon^2L^2 + 2i\epsilon^3L^3 + 2\epsilon^4L^4\dots$.

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