Fourier transform and wavelet approaches to the path integral formulation

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October 1, 2023

Abstract

We calculate energies and wavefunctions of several systems using the path integral formulation of quantum physics. The systems considered are one-dimensional and three-dimensional harmonic oscillators and hydrogen atom in one and three dimensions. We represent the time-evolution operator as matrix in a basis consisting of Deslauriers–Dubuc or Daubechies wavelets. We use Trotter kernels and we also develop an own approximation for the path integral kernel. For the one-dimensional harmonic oscillator we use the exact kernel, too. We also develop a method to calculate wavefunctions with the path integral formulation.

Keywords: path integral, wavelet, harmonic oscillator, hydrogen atom, quantum physics, Fourier transform

1 Introduction

The path integral formulation was developed by Richard Feynman in 1948. It generalizes the action principle of classical mechanics. In path integral formulation the transient state at time t of a quantum mechanical system is obtained from the initial state by formula

$$\Psi(\mathbf{y}, t) = \int e^{\mathrm{i}S[\mathbf{x},\dot{\mathbf{x}}]}\psi_0(\mathbf{x}(t))\mathcal{D}\mathbf{x}. \tag{1}$$

Here the integration is done over all paths beginning with $\mathbf{x}(0) = \mathbf{y}$, the action is given by

$$S[\mathbf{x}, \dot{\mathbf{x}}] = \int L(\mathbf{x}(t), \dot{\mathbf{x}}(t))dt, \tag{2}$$

$L(\mathbf{x}(t), \dot{\mathbf{x}}(t))$ is the Lagrangian of the system, and ψ_0 is the initial state. See [1] for an introduction to the path integral formulation.

The method is often applied by using an imaginary time variable [2]. Ruokosenmäki and Rantala [3, 2] have developed a real-time diffusion method for the path integral formulation. Ruokosenmäki et al. [4] and Gholizadehkalkhoran et al. [5] have also used the path integral method for the calculation of the Hooke's atom. Svensson [6] discusses the computation of the hydrogen atom with the

path integral method. Ho and Inomata [7] and Steiner [8] present an exact treatment of the hydrogen atom with path integral formulation. Path integral treatment of the quantum mechanical harmonic oscillator has been given for example by Ruokosenmäki and Rantala [3].

Wavelets are a basis function set constructed by dilatations and translations of so called mother scaling function and mother wavelet. Mathematical theory of interpolating wavelets has been developed by Chui and Li [9] and Donoho [10]. Höynälänmaa [11] has generalized these results for the multivariate case. Goedecker [12] gives an application-oriented introduction to interpolating wavelets. Höynälänmaa et al. [13] have made Hartree–Fock calculations of atoms using an interpolating wavelet basis. Höynälänmaa and Rantala [14] have also made three-dimensional Hartree-Fock and Density Functional Theory calculations for some atoms and two-atom molecules.

We use the Deslauriers-Dubuc interpolating wavelets [15, 16] in this article. We use atomic units ($e = m_e = \hbar = 4\pi\varepsilon_0 = 1$) and the unitary angular frequency definition of the Fourier transform throughout this article. We abbreviate "atomic units" by a.u and units "Hartree" and "Bohr" by Ha and B. This research did not receive any specific grant from funding agencies in the public, commercial, or not-for-profit sectors.

2 Path Integral Formulation

The time-evolution operator defines the evolution of quantum mechanical system [1]:

$$\Psi(\mathbf{x}, t_b) = \hat{U}(t_b, t_a)\Psi(\mathbf{x}, t_a). \tag{3}$$

For a stationary system it is given by

$$\hat{U}(t_b, t_a) = \exp(-\mathrm{i}(t_b - t_a)\hat{H}) \tag{4}$$

where $\hat{H}$ is the Hamiltonian operator of the system. The time evolution of an eigenstate of a stationary system is given by

$$\Psi_a(\mathbf{x}, t) = \exp(-\mathrm{i}E_a t)\psi_a(\mathbf{x}) \tag{5}$$

where ψ_a is an eigenstate of the time-independent Hamiltonian and E_a is its energy.

The time-evolution operator can be represented as [1]

$$\hat{U}(t_b, t_a)\Psi_a = \int_{\mathbb{R}^d} K(\mathbf{x}_b, t_b; \mathbf{x}_a, t_a)\Psi_a(\mathbf{x}_a, t_a)d\mathbf{x}_a \tag{6}$$

where d is the dimensionality of the system (1, 2, or 3) and function K is called the kernel. In path integral formulation the kernel is given by

$$K(\mathbf{x}_b, t_b; \mathbf{x}_a, t_a) = \lim_{N\to\infty} \sqrt{\frac{m}{2\pi\mathrm{i}\epsilon}}^{Nd} \int_{\mathbb{R}^d} \cdots \int_{\mathbb{R}^d} \exp\left(\mathrm{i}S_N\right) d\mathbf{x}_1 \cdots d\mathbf{x}_{N-1}. \tag{7}$$

For a one-particle system the quantity S_N is given by [17]

$$S_N = \epsilon \sum_{n=1}^{N} \left(\frac{m}{2} \left(\frac{\mathbf{x}_n - \mathbf{x}_{n-1}}{\epsilon} \right)^2 - V(x_n, t_n) \right) \tag{8}$$

and

$$\epsilon = \frac{t_b - t_a}{N}. \tag{9}$$

We also define $\Delta t = t_b - t_a$. The Trotter kernel is an approximation of the path-integral kernel given by [3]

$$\begin{aligned} K(\mathbf{x}_b, \mathbf{x}_a; \Delta t) &= \left(\frac{m}{2\pi \mathsf{i} \Delta t}\right)^{d/2} \\ &\exp\left(\mathsf{i}\left(\frac{m}{2\Delta t}|\mathbf{x}_b - \mathbf{x}_a|^2 - \frac{\Delta t}{2}\left(V(\mathbf{x}_b) + V(\mathbf{x}_a)\right)\right)\right). \end{aligned} \tag{10}$$

3 Stationary State Energies and Wavefunctions

Fourier transform has been used to determine the energy spectrum of a quantum mechanical system with path integral formulation e.g. by Gholizadehkalkhoran et al. [5].

A stationary state ψ of a quantum mechanical system can be represented by

$$\psi(\mathbf{x}) = \sum_{k=0}^{\infty} c_k f_k(\mathbf{x}) \tag{11}$$

where functions f_k are the eigenstates of the Hamiltonian operator of the system and c_k are complex numbers. The time evolution of the stationary states is given by

$$\Psi(\mathbf{x}, t) = \sum_{k=0}^{\infty} c_k \exp(-\mathsf{i} E_k t) f_k(\mathbf{x}) \tag{12}$$

where E_k are the energies of the eigenstates. Suppose that we have a fixed point $\mathbf{x}_0 \in \mathbb{R}^d$ and define $g(t) := \Psi(\mathbf{x}_0, t)$. By making a Fourier transform we obtain

$$\hat{g}(\omega) = \frac{1}{\sqrt{2\pi}} \int_{t=-\infty}^{\infty} g(t) \exp(-\mathsf{i}\omega t) dt \tag{13}$$

$$= \frac{1}{\sqrt{2\pi}} \sum_{k=0}^{\infty} c_k f_k(\mathbf{x}_0) \int_{t=-\infty}^{\infty} \exp(-\mathsf{i} E_k t) \exp(-\mathsf{i}\omega t) dt \tag{14}$$

$$= \sqrt{2\pi} \sum_{k=0}^{\infty} c_k f_k(\mathbf{x}_0) \delta(\omega + E_k). \tag{15}$$

Thus we may compute the eigenenergies of the system from the Fourier spectrum of function g.

Suppose that we have a stationary system with initial state $\psi_i(\mathbf{x}) = \Psi(\mathbf{x}, t_i)$ and final state $\psi_f(\mathbf{x}) = \Psi(\mathbf{x}, t_f)$ and assume that the time interval $\Delta t := t_b - t_a$ is small. We have

$$\psi_f(\mathbf{x}) - \psi_i(\mathbf{x}) = \left(\exp(-\mathsf{i} E t) - 1\right) \psi_i(\mathbf{x}) \approx -\mathsf{i} E t \psi_i(\mathbf{x}) \tag{16}$$

from which we obtain

$$E \approx -\frac{1}{\Delta t} \mathrm{Im} \frac{\psi_f(\mathbf{x}) - \psi_i(\mathbf{x})}{\psi_i(\mathbf{x})} \tag{17}$$

and

$$\langle E\rangle \approx -\frac{1}{\Delta t}\mathrm{Im}\int_{\mathbb{R}^d}\left(\psi_f(\mathbf{x})-\psi_i(\mathbf{x})\right)\left(\psi_i(\mathbf{x})\right)^* d\mathbf{x}. \tag{18}$$

The initial function of the time evolution should be chosen so that it has a broad Fourier spectrum and it should also contain both even and odd terms. So we chose to approximate the sum of delta function and its derivative at the origin with a scaling function centred at the origin and its derivative in the one-dimensional case. In some calculations we use function $-\varphi_{j_{\min},-1}+\varphi_{j_{\min},1}$ instead of the derivative. In three dimensions we use the tensor products of functions $(-1-\mathsf{i})\varphi_{j_{\min},-1}+(1+\mathsf{i})\varphi_{j_{\min},0}+(1+\mathsf{i})\varphi_{j_{\min},1}$.

We use the method described in [18, section 2] to compute the continuous Fourier transform. We have also generalized it into three dimensions.

Let $\mathbf{x}_j$, $j=1,\ldots,N$ be the points where we calculate the wavefunction of state k. Let $g_j(t):=\Psi(\mathbf{x}_j,t)$ and ΔE be the spacing between points in the Fourier spectrum $\hat{g}_j(E)$. We fit the peak k to the Lorentzian distribution

$$L(E)=\frac{1}{\pi}\frac{\gamma}{(E+E_k)^2+\gamma^2}. \tag{19}$$

Define

$$p_{k,j}=\left|\hat{g}_j(-E_k)\right|^2, \tag{20}$$

$$p'_{k,j}=\frac{1}{2}\left(\left|\hat{g}_j(-E_k+\Delta E)\right|^2+\left|\hat{g}_j(-E_k-\Delta E)\right|^2\right), \tag{21}$$

and

$$L_{k,j}(E)=\frac{1}{\pi}\frac{\gamma_{k,j}}{(E+E_k)^2+\gamma_{k,j}^2}. \tag{22}$$

Note that $\left|\hat{g}_j(E)\right|^2$ is the Fourier transform of the autocorrelation function of $g_j(t)$ multiplied by a constant. Let $d_{k,j}=\left|c_k f_k(\mathbf{x}_j)\right|^2$ be the undefined variables. We now set

$$p_{k,j}=d_{k,j}L_{k,j}(-E_k)=d_{k,j}\frac{1}{\pi}\frac{1}{\gamma_{k,j}} \tag{23}$$

and

$$p'_{k,j}=d_{k,j}L_{k,j}(-E_k+\Delta E)=d_{k,j}\frac{1}{\pi}\frac{\gamma_{k,j}}{\Delta E^2+\gamma_{k,j}^2}. \tag{24}$$

It follows that

$$d_{k,j}=\pi\gamma_{k,j}p_{k,j} \tag{25}$$

where

$$\gamma_{k,j}=\sqrt{\frac{q_{k,j}}{1-q_{k,j}}}\,|\Delta E| \tag{26}$$

and

$$q_{k,j}=\frac{p'_{k,j}}{p_{k,j}}. \tag{27}$$

4 Approximation of the Path Integral Kernel

We assume that the potential V does not depend on time. We approximate the kernel by setting $N = 2$ and we get

$$K_2(\mathbf{x}_b, \mathbf{x}_a; \epsilon) := \left(\frac{m}{2\pi \mathsf{i}\epsilon}\right)^d \int_{\mathbb{R}^d} \exp\left(\mathsf{i}S_2\right) d\mathbf{x}_1. \tag{28}$$

We have

$$K_2(\mathbf{x}_b, \mathbf{x}_a; \epsilon) = \left(\frac{m}{2\pi \mathsf{i}\epsilon}\right)^d I \tag{29}$$

where

$$\begin{aligned}
I &:= \int_{\mathbf{x}_1 \in \mathbb{R}^d} \exp(\mathsf{i}S_2) d\mathbf{x}_1 && (30)\\
&= \int_{\mathbf{x}_1 \in \mathbb{R}^d} \exp\left(\mathsf{i}\epsilon \left(\frac{m}{2}\left(\frac{\mathbf{x}_1 - \mathbf{x}_a}{\epsilon}\right)^2 - V(\mathbf{x}_1)\right.\right. \\
&\quad \left.\left. + \frac{m}{2}\left(\frac{\mathbf{x}_b - \mathbf{x}_1}{\epsilon}\right)^2 - V(\mathbf{x}_b)\right)\right) d\mathbf{x}_1 && (31)\\
&= \exp\left(\mathsf{i}\left(\frac{m}{2\epsilon}\left(\mathbf{x}_b^2 + \mathbf{x}_a^2\right) - \epsilon V(\mathbf{x}_b)\right)\right) \\
&\quad \int_{\mathbf{x}_1 \in \mathbb{R}^d} \exp\left(\mathsf{i}\left(\frac{m}{\epsilon}\mathbf{x}_1^2 - \epsilon V(\mathbf{x}_1)\right)\right) \exp\left(-\mathsf{i}\frac{m}{\epsilon}(\mathbf{x}_b + \mathbf{x}_a)\cdot \mathbf{x}_1\right) d\mathbf{x}_1 && (32)\\
&= \sqrt{2\pi}^d \exp\left(\mathsf{i}\left(\frac{m}{2\epsilon}\left(\mathbf{x}_b^2 + \mathbf{x}_a^2\right) - \epsilon V(\mathbf{x}_b)\right)\right) \hat{h}\left(\frac{m}{\epsilon}(\mathbf{x}_b + \mathbf{x}_a)\right) && (33)
\end{aligned}$$

and

$$h(\mathbf{x}_1) := \exp\left(\mathsf{i}\left(\frac{m}{\epsilon}\mathbf{x}_1^2 - \epsilon V(\mathbf{x}_1)\right)\right). \tag{34}$$

Now

$$K_2(\mathbf{x}_b, \mathbf{x}_a; \epsilon) = \left(\frac{m}{2\pi \mathsf{i}\epsilon}\sqrt{2\pi}\right)^d \exp\left(\mathsf{i}\left(\frac{m}{2\epsilon}\left(\mathbf{x}_b^2 + \mathbf{x}_a^2\right) - \epsilon V(\mathbf{x}_b)\right)\right) \hat{h}\left(\frac{m}{\epsilon}(\mathbf{x}_b + \mathbf{x}_a)\right). \tag{35}$$

We call this kernel the *midpoint kernel*.

If function h is radially symmetric (i.e. the potential is radially symmetric) we have

$$\hat{h}(\mathbf{k}) = \frac{\mathsf{i}}{2k}\left(\hat{f}(k) - \hat{f}(-k)\right), \tag{36}$$

where $f(r) = r h_{\mathrm{rad}}(|r|)$ and $h(\mathbf{r}) = h_{\mathrm{rad}}(|\mathbf{r}|)$. Note that the Fourier transform of f in equation (36) is one-dimensional.

5 Quantum Harmonic Oscillator and Hydrogen-like Atom

The potential of the one-dimensional harmonic oscillator is

$$V(x) = \frac{m\omega_0^2}{2} x^2 \tag{37}$$

where m is the mass of the particle and ω_0 is the angular frequency. The potential of the isotropic three-dimensional harmonic oscillator is

$$V(\mathbf{x}) = \frac{m\omega_0^2}{2}|\mathbf{x}|^2. \tag{38}$$

The kernel for the one-dimensional harmonic oscillator can be computed exactly [1]. We have

$$K(x_b, x_a; t) = \left(\frac{m\omega_0}{2\pi\mathrm{i}\sin(\omega_0 t)}\right)^{1/2} \exp(\mathrm{i}S_{\mathrm{cl}}), \tag{39}$$

where S_{cl} is the classical action given by

$$S_{\mathrm{cl}} = \frac{m\omega_0}{2\sin(\omega_0 t)}\left((x_b^2 + x_a^2)\cos(\omega_0 t) - 2x_b x_a\right). \tag{40}$$

By substituting the potential of the one-dimensional harmonic oscillator to equation (34) we obtain

$$h(x_1) = \exp\left(\mathrm{i}\frac{m}{\epsilon}\left(1 - \frac{\epsilon^2\omega_0^2}{2}\right)x_1^2\right). \tag{41}$$

Define

$$a := \frac{m}{\epsilon}\left(1 - \frac{\epsilon^2\omega_0^2}{2}\right) \tag{42}$$

and assume that $a > 0$. Now

$$\hat{h}(k) = \frac{1}{2}(1+\mathrm{i})\frac{1}{\sqrt{a}}\exp\left(-\mathrm{i}\frac{k^2}{4a}\right). \tag{43}$$

Similarly, in the three-dimensional case we have

$$\hat{h}(\mathbf{k}) = \frac{1}{4}(-1+\mathrm{i})a^{-3/2}\exp\left(-\mathrm{i}\frac{k^2}{4a}\right) \tag{44}$$

using equation (36).

The potential of a hydrogen-like atom is

$$V(x) = -\frac{Z}{|x|} \tag{45}$$

in one dimension and

$$V(\mathbf{x}) = -\frac{Z}{|\mathbf{x}|} \tag{46}$$

in three dimensions. Here Z is the atomic number.

6 Wavelet Bases

6.1 Interpolating Wavelets

We construct the basis function set in the same way as in [14, section 3]. We assume that φ is some Deslauriers–Dubuc mother scaling function [9, 10, 11, 15,

16] and d is the dimensionality of the domain $\mathbb{R}^d$. We use only bases with one or two resolution levels in this article. Constant $j_{\min}$ is the minimum resolution level in the basis, see [14]. We define G to be the whole basis, $G = G_{j_{\min}}$ or $G = G_{j_{\min}} \cup G_{j_{\min}+1}$.

The interpolating mother scaling function can be represented as [9, 11]

$$\varphi(x) = \sum_{\alpha \in \mathbb{Z}} s[\alpha] \varphi(2^J x - \alpha) \tag{47}$$

where J is some nonnegative integer and $s[\alpha]$, $\alpha \in \mathbb{Z}$, are constants that depend on the mother scaling function and J. We define $s_0[\alpha]$ to be the coefficients for J and $s_1[\alpha]$ for $J-1$. We now have

$$\eta_{j_{\min},k}(2^{-J-j_{\min}} p) = s_0[p - 2^J k] \tag{48}$$

for all $p \in \mathbb{Z}$,

$$\eta_{j_{\min}+1,k}(2^{-J-j_{\min}} p) = s_0[p - 2^{J-1} k] \tag{49}$$

for all $p \in \mathbb{Z}$ and k even integer, and

$$\eta_{j_{\min}+1,k}(2^{-J-j_{\min}} p) = s_1[p - 2^{J-1} k] \tag{50}$$

for all $p \in \mathbb{Z}$ and k odd integer. We also have

$$\tilde{\eta}_{j_{\min},\ell} = \tilde{\varphi}_{j_{\min},\ell} = \delta(\cdot - 2^{-j_{\min}} \ell) \tag{51}$$

for all $\ell \in \mathbb{Z}$,

$$\tilde{\eta}_{j_{\min}+1,\ell} = \delta(\cdot - 2^{-j_{\min}-1} \ell) = \sum_{\beta \in \mathbb{Z}} \tilde{h}_\beta \delta(\cdot - 2^{-j_{\min}-1}(\beta + \ell)) \tag{52}$$

for all $\ell \in 2\mathbb{Z}$, and

$$\tilde{\eta}_{j_{\min}+1,\ell} = \sum_{\beta \in \mathbb{Z}} \tilde{g}_\beta \delta(\cdot - 2^{-j_{\min}-1}(\beta + \ell - 1)) \tag{53}$$

for all $\ell \in 2\mathbb{Z} + 1$.

The matrix of the time evolution operator in the interpolating wavelet basis is

$$K_{\mathbf{r},\mathbf{q}} = \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \tilde{\zeta}_{\mathbf{r}}(\mathbf{y}) K(\mathbf{y}, \mathbf{x}) \zeta_{\mathbf{q}}(\mathbf{x}) d\mathbf{x} d\mathbf{y}. \tag{54}$$

Note that the dual wavelets $\tilde{\zeta}_{\mathbf{r}}$ are finite sums of delta distributions and consequently the integration over $\mathbf{y}$ is actually a weighted sum of values of the function

$$\int_{\mathbb{R}^d} K(\mathbf{y}, \mathbf{x}) \zeta_{\mathbf{q}}(\mathbf{x}) d\mathbf{x}$$

in finite number of points $\mathbf{y}$. When $\mathbf{r} = 2^{-j_{\min}} \ell \in G_{j_{\min}}$ we have

$$K_{\mathbf{r},\mathbf{q}} = \int_{\mathbb{R}^d} K(2^{-j_{\min}} \ell, \mathbf{x}) \zeta_{\mathbf{q}}(\mathbf{x}) d\mathbf{x}. \tag{55}$$

In one-dimensional case the integral over x is approximated by

$$\int_{\mathbb{R}} K(y, x) \zeta_q(x) dx \approx 2^{-j_{\min}-J} \sum_{p \in \mathbb{Z}} K(y, 2^{-j_{\min}-J} p) s_{t(q)}(p - 2^{J-t(q)} k) \tag{56}$$

where $k \in \mathbb{Z}$, $q = 2^{-j_{\min}} k \in G_{j_{\min}}$ or $q = 2^{-j_{\min}-1} k \in G_{j_{\min}+1}$, and

$$t(q) := \begin{cases} 1 & \text{if } q \in G_{j_{\min}+1} \\ 0 & \text{if } q \in G_{j_{\min}}. \end{cases} \tag{57}$$

For the three-dimensional case define

$$t_i(\mathbf{q}) := \begin{cases} 1 & \text{if } \mathbf{q} \in G_{j_{\min}+1} \text{ and } 2^{j_{\min}+1}\mathbf{q}[i] \text{ odd} \\ 0 & \text{otherwise} \end{cases} \tag{58}$$

for $i = 1, 2, 3$ and $\mathbf{t}(\mathbf{q}) := (t_1(\mathbf{q}), t_2(\mathbf{q}), t_3(\mathbf{q})$. Define also

$$s_{\mathbf{t}}(\mathbf{z}) := s_{t[1]}(\mathbf{z}[1]) s_{t[2]}(\mathbf{z}[2]) s_{t[3]}(\mathbf{z}[3]). \tag{59}$$

Now we can approximate

$$\int_{\mathbb{R}^3} K(\mathbf{y}, \mathbf{x}) \zeta_{\mathbf{q}}(\mathbf{x}) d\mathbf{x} \approx 2^{-3(j_{\min}+J)} \sum_{\mathbf{p} \in \mathbb{Z}^3} K(\mathbf{y}, 2^{-j_{\min}-J}\mathbf{p}) s_{\mathbf{t}(\mathbf{q})}(\mathbf{p} - \mathbf{w} \cdot \mathbf{k}) \tag{60}$$

where $\mathbf{k} \in \mathbb{Z}^3$ and $\mathbf{q} = 2^{-j_{\min}}\mathbf{k} \in G_{j_{\min}}$ or $\mathbf{q} = 2^{-j_{\min}-1}\mathbf{k} \in G_{j_{\min}+1}$, and $\mathbf{w} := (2^{J-t_1(\mathbf{q})}, 2^{J-t_2(\mathbf{q})}, 2^{J-t_3(\mathbf{q})})^T$. We pick some value $J_0 \geq 2$ and for $\mathbf{r} \in G_{j_{\min}+1}$ we use value $J = J_0 - 1$ in equation (47) and $J = J_0$ otherwise. The lower accuracy is used because the matrix elements where $\mathbf{q}$ belongs to the finer grid are significantly more complex to compute as the ones in the coarser grid.

We use 8th order Deslauriers–Dubuc wavelets for one-dimensional calculations and 4th order Deslauriers–Dubuc wavelets for three-dimensional calculations.

6.2 Orthonormal Wavelets

See [19] for more information on orthonormal wavelets. We define the basis indices by $I = I_{j_{\min}} \cup I_{j_{\min}+1}$ where $I_j = \{(j, k) : k \in K_j\}$ and K_j is a finite set of integer numbers (usually a range of integers). Now the basis functions are defined by

$$\zeta_{j,k} = \begin{cases} \varphi_{j_{\min},k} = 2^{j/2}\varphi(2^j \cdot -k) & j = j_{\min} \\ \psi_{j-1,k} = 2^{(j-1)/2}\psi(2^{j-1} \cdot -k) & j > j_{\min} \end{cases} \tag{61}$$

where $(j, k) \in I$, φ is the mother scaling function of the wavelet family, and ψ is the mother wavelet of the wavelet family. In order to compute the values of the orthonormal wavelets we use the represention

$$\varphi(x) = 2^{J/2} \sum_{\alpha \in \mathbb{Z}} w[\alpha] \varphi(2^J x - \alpha) \tag{62}$$

where J is some nonnegative integer and $w[\alpha]$, $\alpha \in \mathbb{Z}$, are constants that depend on the mother scaling function and J. The matrix elements of the time-evolution operator are given by

$$K_{j,k,j',k'} = \int_{\mathbb{R}} \int_{\mathbb{R}} \zeta_{j,k}(y) K(y, x) \zeta_{j',k'}(x) dx dy \tag{63}$$

with orthonormal wavelets. We use the 20th order Daubechies wavelets in this study. We use only one-dimensional orthonormal wavelets.

7 Application to the Harmonic Oscillator and Hydrogen Atom

Unless otherwise stated the calculations use Deslauriers–Dubuc wavelets.

We make calculations for the one-dimensional harmonic oscillator with the exact kernel, Trotter kernel, and midpoint kernel. We compute all these system with both one and two resolution levels of the basis functions for $\Delta t = 1.0$ a.u. and one resolution level for $\Delta t = 0.5$ a.u. and $\Delta t = 0.25$ a.u. The mass of the particle is 1 a.u. and the angular frequency 0.1 radians. All these calculations yield the ground state energy 0.050265 Ha and first excited state 0.150796 Ha or 0.149226 Ha. We use the basis $(1/4)\{-48, \ldots, 48\}$ for one-level calculations and $(1/4)\{-48, \ldots, 48\} \cup (1/8)\{-5, \ldots, 5\}$ for two-level calculations. We use scaling function resolution $J = 3$. The energy spectrum for the exact kernel is plotted in Fig. 1 and for the midpoint kernel in Fig. 2. Both of these calculations use two resolution levels. The wavefunction of the one-dimensional harmonic oscillator calculated with the method described in section 3 is plotted in Fig. 3.

When the Deslauriers–Dubuc (interpolating) wavelets are used for the hydrogen atom the calculations work for parameter $\Delta t = 1$ a.u. but not for $\Delta t = 0.5$ a.u. So we calculated this system with Daubechies (orthonormal) wavelets using both Trotter and midpoint kernels. For one resolution level calculations we use the basis $\{(2, -48), \ldots, (2, 48)\}$ and for the two-level calculations $\{(1, -24), \ldots, (1, 24)\} \cup \{(2, -6), \ldots, (2, 6)\}$ We set the mother scaling function resolution to $J = 5$. The resulting ground state energies are presented in Table 1. It can be seen that for the same time parameter the midpoint kernel yields usually better energy compared to the Trotter kernel but the Trotter kernel accepts smaller time parameters. The best energy for the Trotter kernel is $E_0 = -0.502655$ Ha and if the energies smaller that the exact energy are neglected we get $E_0 = -0.494801$ Ha. The best energy for the midpoint kernel is $E_0 = -0.496372$ Ha. The best energy spectrum for the Trotter kernel is plotted in Fig. 4 and for the midpoint kernel in Fig. 5. The radial probability density function of the hydrogen atom calculated in one dimension with the the method described in section 3 is plotted in Fig. 6.

We make calculations for the three-dimensional harmonic oscillator using the midpoint kernel and the Trotter kernel. The mass of the particle is 1 a.u. and the angular frequency 0.1 radians. We use basis $\{-10, \ldots, 10\}^3$ and mother scaling function resolution $J = 2$. The resulting ground state energy for the midpoint kernel is $E_0 = 0.150796$ Ha and the first excited state $E_1 = 0.249757$ Ha for $\Delta t = 4.0$ a.u.. For $\Delta t = 2.0$ a.u. the energies are $E_0 = 0.150796$ Ha and $E_1 = 0.251327$ Ha. The energy spectrum for $\Delta t = 2.0$ a.u. is plotted in Fig. 7. For the Trotter kernel the energies are $E_0 = 0.150796$ Ha and $E_1 = 0.251327$ Ha for both $\Delta t = 4.0$ a.u. and $\Delta t = 2.0$ a.u..

We make three-dimensional calculations of the hydrogen atom using the midpoint kernel and the Trotter kernel. The basis function set is $(1/2)\{-9, \ldots, 9\} \cup (1/4)\{-4, \ldots, 4\}$. The function $\hat{h}(\mathbf{k})$ for the midpoint kernel is calculated with formula (36). We have to invert the sign of the midpoint kernel (35) in order to get the energy computation to work. We get energy $E = -0.474380$ Ha for the midpoint kernel with parameter $\Delta t = 2.0$ a.u. and value $\Delta t = 1.5$ a.u. does not yield reasonable results. For the Trotter kernel we get $E = -0.477522$ Ha with parameter $\Delta t = 0.2$ a.u. and value $\Delta t = 0.125$ a.u. does not give reasonable

Table 1: Energies from the one-dimensional calculations of the hydrogen atom.

kernel	res. levels	Δt	E_0 (Ha)	E_1 (Ha)
midpoint	1	1	-0.446106	-0.131947
midpoint	2	1	-0.446106	-0.113097
Trotter	1	1	-0.402124	-0.106814
Trotter	2	1	-0.402124	-0.106814
midpoint	1	0.5	-0.471239	-0.119381
midpoint	2	0.5	.0.471239	-0.119310
Trotter	1	0.5	-0.446106	-0.113097
Trotter	2	0.5	-0.452389	-0.113097
midpoint	1	0.25	-0.490088	-0.119381
midpoint	2	0.25	-0.490088	-0.119381
Trotter	1	0.25	-0.471239	-0.119381
Trotter	2	0.25	-0.477522	-0.119381
midpoint	1	0.20	-0.490088	-0.131947
midpoint	2	0.20	-0.483805	-0.144513
Trotter	1	0.20	-0.477522	-0.119381
Trotter	2	0.20	-0.483805	-0.119381
midpoint	1	0.125	-0.496372	-0.113097
midpoint	2	0.125	-	-
Trotter	1	0.125	-0.490088	-0.119381
Trotter	2	0.125	-0.490088	-0.119381
midpoint	1	0.1	-0.510509	-
Trotter	1	0.1	-0.494801	-0.117810
Trotter	2	0.1	-0.494801	-0.117810
Trotter	1	0.0625	-0.490088	-0.125664
Trotter	2	0.0625	-	-
midpoint	1	0.05	-	-
Trotter	1	0.03125	-0.502655	-0.125664
Trotter	1	0.03	-	-

results.

Note that we get exactly same energy values for many different calculations because the energy spectrum $\hat{g}(-E)$ is approximated by the Discrete Fourier Transform, for which the energy values are discrete. Ruokosenmäki [17] has discussed the behavior of the path integral kernel with small values of Δt, too. It turned out that when the time step parameter Δt is the same the midpoint kernel gives usually better energy than the Trotter kernel for the hydrogen atom (one and three dimensions) but the Trotter kernel accepts smaller values for Δt. The two kernels yield approximately the same energy for the harmonic oscillator.

8 Acknowledgments

The author thanks professor Tapio T. Rantala for proofreading the article.

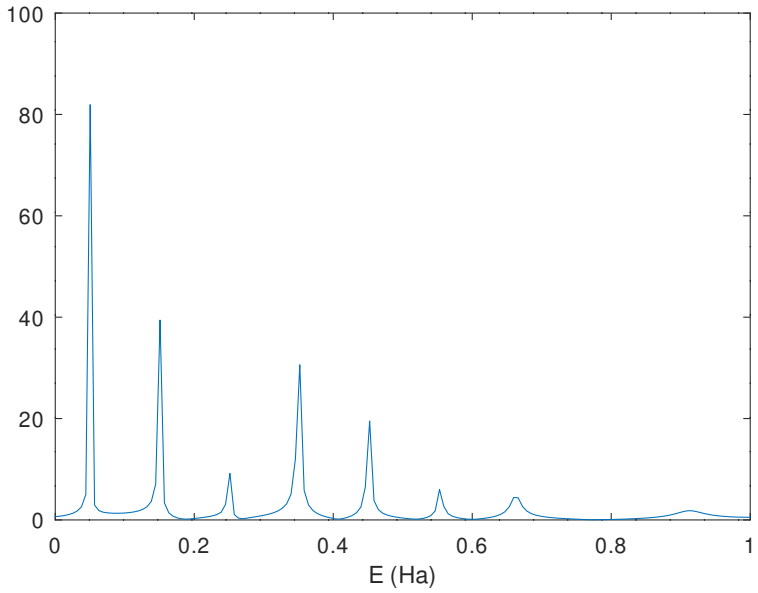

Figure 1: Energy spectrum of the one-dimensional harmonic oscillator computed with the exact kernel.

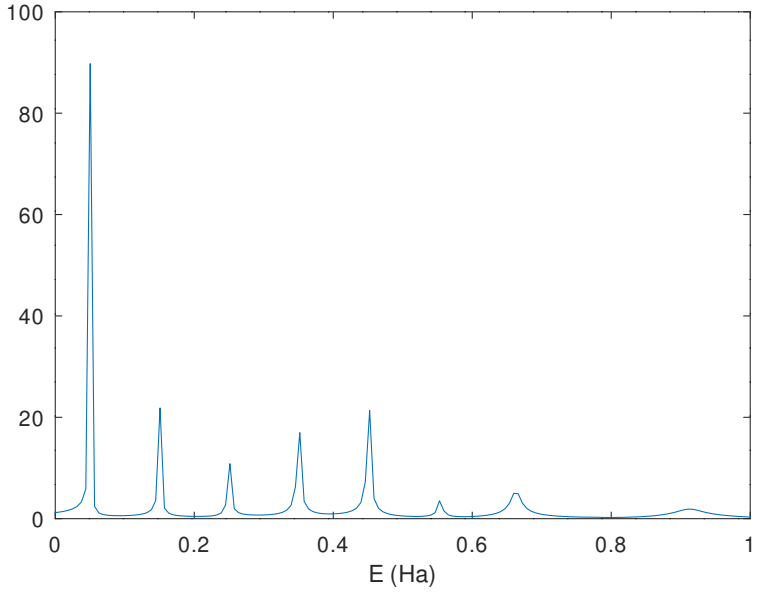

Figure 2: Energy spectrum of the one-dimensional harmonic oscillator computed with the midpoint kernel.

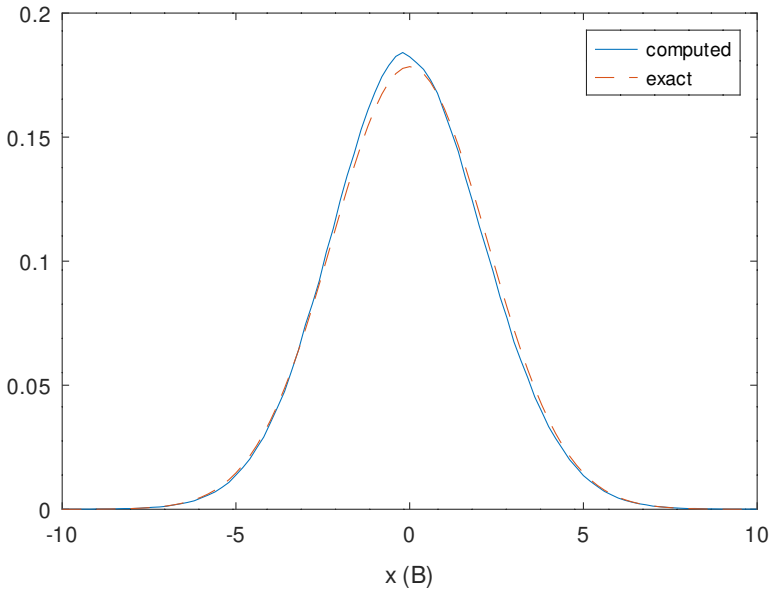

Figure 3: Probability density function $|\psi(x)|^2$ of the one-dimensional harmonic oscillator computed with the exact kernel.

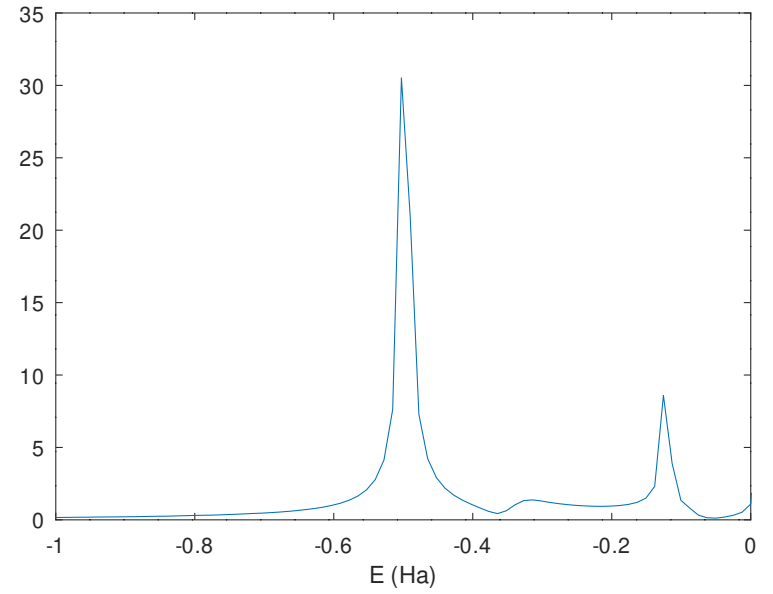

Figure 4: Energy spectrum of the hydrogen atom computed with the Trotter kernel in one dimension.

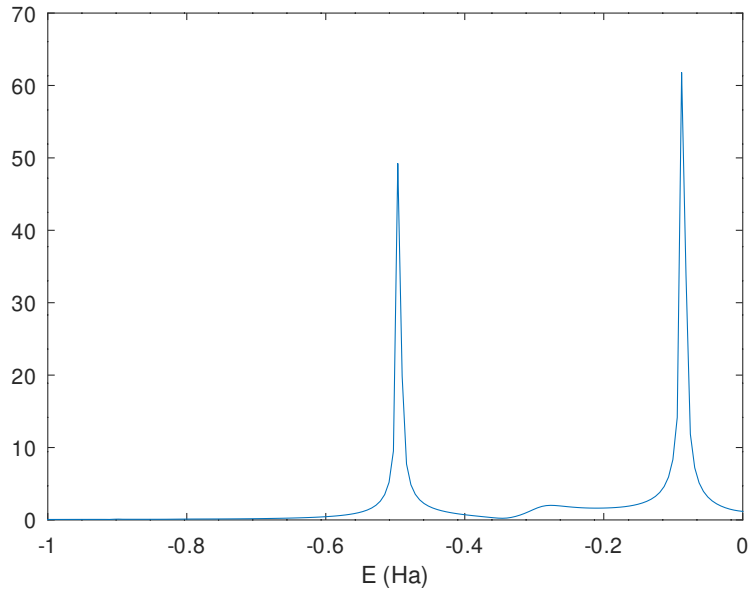

Figure 5: Energy spectrum of the hydrogen atom computed with the midpoint kernel in one dimension.

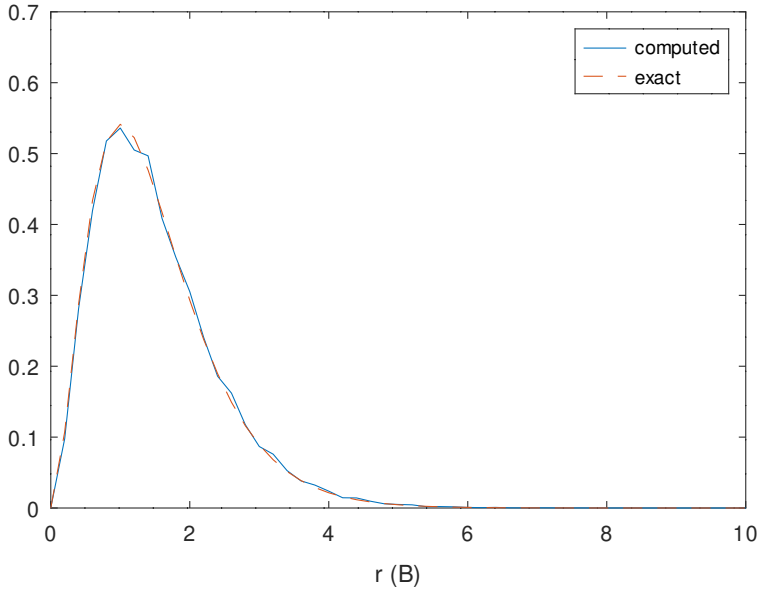

Figure 6: Radial probability density function $|P_{1s}(r)|^2$ of the hydrogen atom computed with the midpoint kernel in one dimension.

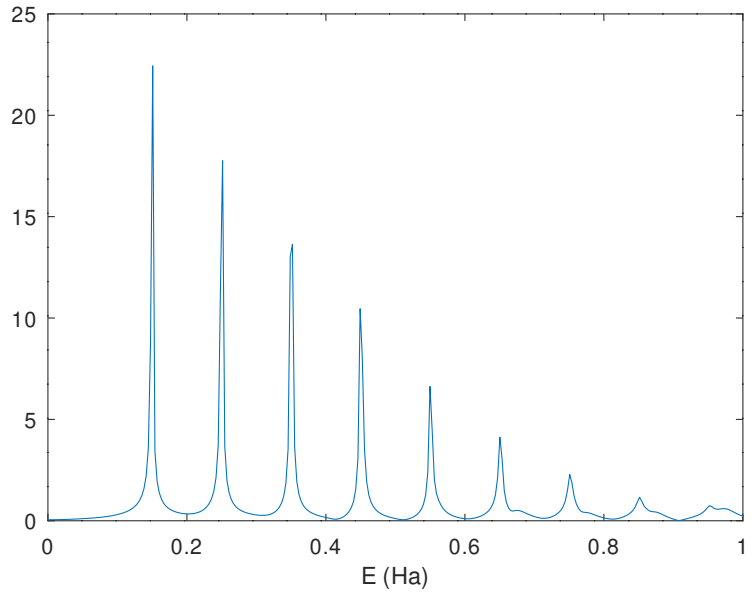

Figure 7: Energy spectrum of the three-dimensional harmonic oscillator calculated with the midpoint kernel.

References

[1] Richard P. Feynman and Albert R. Hibbs and Daniel F. Styer. *Quantum Mechanics and Path Integrals*. Courier Corporation, 2010.

[2] Ilkka Ruokosenmäki and Tapio T. Rantala. "Real-Time Diffusion Monte Carlo Method". In: *Commun. Comput. Phys.* 25.2 (2019), pp. 347–360. DOI: 10.4208/cicp.OA-2018-0048.

[3] Ilkka Ruokosenmäki and Tapio T. Rantala. "Numerical Path Integral Approach to Quantum Dynamics and Stationary Quantum States". In: *Commun. Comput. Phys.* 18.1 (2015), pp. 91–103. DOI: 10.4208/cicp.180914.161214a.

[4] Ilkka Ruokosenmäki et al. "Numerical path integral solution to strong Coulomb correlation in one dimensional Hooke's atom". In: *Computer Physics Communications* 210 (2017), pp. 45–53. DOI: 10.1016/j.cpc.2016.09.012.

[5] Hossein Gholizadehkalkhoran, Ilkka Ruokosenmäki, and Tapio T. Rantala. "Eigenstates and dynamics of Hooke's atom: Exact results and path integral simulations". In: *J. Math. Phys.* 59 (2018), p. 052104. DOI: 10.1063/1.5028503.

[6] Anders Svensson. "Path Integral for the Hydrogen Atom: Solutions in two and three dimensions". B. S. Thesis. 2016. URL: http://www.diva-portal.se/smash/get/diva2:947133/FULLTEXT01.pdf.

[7] Roger Ho and Akira Inomata. "Exact-Path-Integral Treatment of the Hydrogen Atom". In: *Phys. Rev. Lett.* 48 (4 Jan. 1982), pp. 231–234. DOI:

10.1103/PhysRevLett.48.231. URL: https://link.aps.org/doi/10.1103/PhysRevLett.48.231.

[8] F. Steiner. "Exact path integral treatment of the hydrogen atom". In: *Physics Letters A* 106.8 (1984), pp. 363–367. ISSN: 0375-9601. DOI: https://doi.org/10.1016/0375-9601(84)90917-4. URL: https://www.sciencedirect.com/science/article/pii/0375960184909174.

[9] Charles K. Chui and Chun Li. "Dyadic Affine Decompositions and Functional Wavelet Transforms". In: *SIAM J. Math. Anal.* 27.3 (1996), pp. 865–890. DOI: 10.1137/0527046.

[10] David L. Donoho. *Interpolating Wavelet Transforms*. Tech. rep. 408. Department of Statistics, Stanford University, 1992.

[11] Tommi Höynälänmaa. "Multiresolution Analysis for Compactly Supported Interpolating Tensor Product Wavelets". In: *Int. J. Wavelets Multiresolut Inf. Process.* 13.2 (2015), p. 1550010. DOI: 10.1142/S0219691315500101.

[12] S. Goedecker. *Wavelets and their application for the solution of partial differential equations in physics*. Presses Polytechniques et Universitaires Romandes, 1998.

[13] Tommi Höynälänmaa, Tapio T. Rantala, and Keijo Ruotsalainen. "Solution of atomic orbitals in an interpolating wavelet basis". In: *Phys. Rev. E* 70 (2004), p. 066701. DOI: 10.1103/PhysRevE.70.066701.

[14] Tommi Höynälänmaa and Tapio T. Rantala. "Electronic structure calculations with interpolating tensor product wavelet basis". In: *Phys. Rev. E* 108 (2023), p. 025307. DOI: 10.1103/PhysRevE.108.025307.

[15] Serge Dubuc. "Interpolation through an Iterative Scheme". In: *J. Math. Anal. Appl.* 114 (1986), pp. 185–204. DOI: 10.1016/0022-247X(86)90077-6.

[16] Gilles Deslauriers and Serge Dubuc. "Symmetric Iterative Interpolation Processes". In: *Constr. Approx.* 5.1 (1989), pp. 49–68. DOI: 10.1007/BF01889598.

[17] Ilkka Ruokosenmäki. "Real Time Path Integral Simulation Methods for Quantum Particles". PhD thesis. Tampere University, 2019.

[18] David H. Bailey and Paul N. Swarztrauber. "A Fast Method for the Numerical Evaluation of Continuous Fourier and Laplace Transforms". In: *SIAM J. on Scientific Computing* 15.5 (1994), pp. 1105–1110.

[19] I. Daubechies. *Ten Lectures on Wavelets*. CBMS-NSF regional conference series in applied mathematics ; 61. SIAM, 1992. DOI: 10.1137/1.9781611970104.