

# Wavelet basis and Fourier transform approach to the path integral formulation of electron dynamics

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## Abstract

We present a new method for the path integral formulation of electronic structure simulation. The time evolution operator is represented as matrix in a basis consisting of Deslauriers–Dubuc or Daubechies wavelets. We present a new approximation of the path integral kernel and a new method for calculating wavefunctions using the path integral formulation. The new kernel is tested by finding wavefunctions and energies of one-dimensional and three-dimensional harmonic oscillators and hydrogen atom in one and three dimensions.

*Keywords:* path integral, wavelet, quantum chemistry, hydrogen atom, quantum physics, Fourier transform

## 1 Introduction

The path integral formulation of quantum dynamics 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 system is obtained from the initial state  $\Psi(\mathbf{x}_a, t_a)$  by

$$\Psi(\mathbf{x}_b, t_b) = \hat{U}(t_b, t_a)\Psi(\mathbf{x}_a, t_a) = \int_{\mathbb{R}^d} K(\mathbf{x}_b, t_b; \mathbf{x}_a, t_a)\Psi(\mathbf{x}_a, t_a)d\mathbf{x}_a, \quad (1)$$

where  $\hat{U}$  is the time evolution operator and  $d$  is the dimensionality of the system,  $d = 1$ ,  $d = 2$ , or  $d = 3$ . The kernel is given by

$$K(\mathbf{x}_b, t_b; \mathbf{x}_a, t_a) = \int_a^b \exp\left(\frac{i}{\hbar} S[\mathbf{x}, \dot{\mathbf{x}}]\right) \mathcal{D}\mathbf{x}, \quad (2)$$

where the integration is carried out over all paths with  $\mathbf{x}(t_a) = \mathbf{x}_a$  and  $\mathbf{x}(t_b) = \mathbf{x}_b$  and the action is

$$S[\mathbf{x}, \dot{\mathbf{x}}] = \int_{t_a}^{t_b} L(\mathbf{x}(t), \dot{\mathbf{x}}(t))dt, \quad (3)$$

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where  $L(\mathbf{x}(t), \dot{\mathbf{x}}(t))$  is the Lagrangian of the system. See Ref. [1] for more details.

The path-integral method is often applied by using an imaginary time variable [2]. Svensson [3] discusses the computation of the hydrogen atom with the path integral method. Ho and Inomata [4] and Steiner [5] 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 [6].

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 [7] and Donoho [8]. Höynälänmaa [9] has generalized these results for the multivariate case. Goedecker [10] gives an application-oriented introduction to interpolating wavelets. Höynälänmaa et al. [11] have made Hartree–Fock calculations of atoms using an interpolating wavelet basis. Höynälänmaa and Rantala [12] have also made three-dimensional Hartree–Fock and Density Functional Theory calculations using interpolating wavelets for some atoms and two-atom molecules. Orthonormal wavelets are presented e.g. by Daubechies [13].

Here, we use the Deslauriers–Dubuc interpolating wavelets [14, 15] and Daubechies orthonormal wavelets [13]. Also, atomic units ( $e = m_e = \hbar = 4\pi\epsilon_0 = 1$ ) and the unitary angular frequency definition of the Fourier transform are used throughout this article. We abbreviate “atomic units” by a.u. and units “Hartree” and “Bohr” by Ha and B. Also, a stationary wavefunction is denoted by  $\chi$  as the symbol  $\psi$  is used for wavelets.

## 2 Path Integral Formulation

For a stationary system the time evolution operator is given by

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

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

$$\Psi_a(\mathbf{x}, t) = \exp(-iE_a t)\chi_a(\mathbf{x}) \quad (5)$$

where  $\Psi_a$  is an eigenstate of the time-independent Hamiltonian and  $E_a$  is its energy.

In path integral formulation the kernel (2) can be represented [1] as

$$K(\mathbf{x}_b, t_b; \mathbf{x}_a, t_a) = \lim_{N \rightarrow \infty} \sqrt{\frac{m}{2\pi i \epsilon}}^{Nd} \int_{\mathbb{R}^d} \cdots \int_{\mathbb{R}^d} \exp(iS_N) d\mathbf{x}_1 \cdots d\mathbf{x}_{N-1}. \quad (6)$$

For a one-particle system the action  $S_N$  is given by [16]

$$S_N = \epsilon \sum_{n=1}^N \left( \frac{m}{2} \left( \frac{\mathbf{x}_n - \mathbf{x}_{n-1}}{\epsilon} \right)^2 - V(\mathbf{x}_n, t_n) \right) \quad (7)$$

and

$$\epsilon = \frac{t_b - t_a}{N}. \quad (8)$$

We also define  $\Delta t = t_b - t_a$ . The Trotter kernel is an approximation of the path-integral kernel [6] given by

$$K(\mathbf{x}_b, \mathbf{x}_a; \Delta t) = \left( \frac{m}{2\pi i \Delta t} \right)^{d/2} \exp \left( i \left( \frac{m}{2\Delta t} |\mathbf{x}_b - \mathbf{x}_a|^2 - \frac{\Delta t}{2} (V(\mathbf{x}_b) + V(\mathbf{x}_a)) \right) \right). \quad (9)$$

### 3 Wavelet Bases

#### 3.1 Interpolating Wavelets

The basis function set is constructed in the same way as in Ref. [12, section 3]. We assume that  $\varphi$  is some Deslauriers–Dubuc mother scaling function [7, 8, 9, 14, 15] and  $d$  is the dimensionality of the domain  $\mathbb{R}^d$ . The multiresolution analysis for interpolating wavelets may be constructed either in the space of bounded and uniformly continuous functions  $C_u(\mathbb{R}^d)$  or in the space of continuous functions vanishing at infinity  $C_0(\mathbb{R}^d)$ . Both of these spaces use the supremum norm.

The mother scaling function  $\varphi$  satisfies the relation

$$\varphi(x) = \sum_{\mu} h_{\mu} \varphi(2x - \mu) \quad (10)$$

and the mother wavelet is given by  $\psi(x) = \varphi(2x - 1)$ . We assume that the filter  $h_{\mu}$  is finite in this article. This is true at least for Deslauriers–Dubuc wavelets. The doubly indexed scaling functions are given by  $\varphi_{j,k}(x) = \varphi(2^j x - k)$  and the doubly indexed wavelets by  $\psi_{j,k}(x) = \psi(2^j x - k)$ . The dual scaling functions are defined by  $\tilde{\varphi}_{j,k} = 2^j \delta(2^j \cdot - k)$  and the dual wavelets by  $\tilde{\psi}_{j,k} = 2^j \tilde{\psi}(2^j \cdot - k)$  where

$$\tilde{\psi} = 2 \sum_{\nu} \tilde{g}_{\nu} \delta(2 \cdot - \nu) \quad (11)$$

and  $\tilde{g}_{\nu} = (-1)^{\nu-1} h_{1-\nu}$ .

When an interpolating wavelet basis is constructed we select the minimum resolution level  $j_{\min} \in \mathbb{Z}$  and an arbitrary function  $f$  in the space where the MRA is constructed can be represented as

$$f(x) = \sum_k c_{j_{\min},k} \varphi_{j_{\min},k}(x) + \sum_{j=j_{\min}}^{\infty} \sum_k d_{j,k} \psi_{j,k}(x) \quad (12)$$

where  $c_{j_{\min},k} = \langle \tilde{\varphi}_{j_{\min},k}, f \rangle$  and  $d_{j,k} = \langle \tilde{\psi}_{j,k}, f \rangle$ . In practical computations we truncate the basis set to be finite. We also define

$$\psi_{s,j,k}(x) = \begin{cases} \varphi_{j,k}(x); & \text{if } s = 0 \\ \psi_{j,k}(x); & \text{if } s = 1 \end{cases} \quad (13)$$

and

$$\tilde{\psi}_{s,j,k} = \begin{cases} \varphi_{j,k}^{\sim}; & \text{if } s = 0 \\ \psi_{j,k}^{\sim}; & \text{if } s = 1 \end{cases} \quad (14)$$

For the three-dimensional case we define

$$\varphi_{j,\mathbf{k}}(\mathbf{x}) = \varphi_{j,\mathbf{k}[1]}(\mathbf{x}[1]) \varphi_{j,\mathbf{k}[2]}(\mathbf{x}[2]) \varphi_{j,\mathbf{k}[3]}(\mathbf{x}[3]), \quad (15)$$

$$\psi_{\mathbf{s},j,\mathbf{k}}(\mathbf{x}) = \psi_{\mathbf{s}[1],j,\mathbf{k}[1]}(\mathbf{x}[1])\psi_{\mathbf{s}[2],j,\mathbf{k}[2]}(\mathbf{x}[2])\psi_{\mathbf{s}[3],j,\mathbf{k}[3]}(\mathbf{x}[3]), \quad (16)$$

$$\tilde{\varphi}_{j,\mathbf{k}} = \tilde{\varphi}_{j,\mathbf{k}[1]} \otimes \tilde{\varphi}_{j,\mathbf{k}[2]} \otimes \tilde{\varphi}_{j,\mathbf{k}[3]}, \quad (17)$$

$$\tilde{\psi}_{\mathbf{s},j,\mathbf{k}} = \tilde{\psi}_{\mathbf{s}[1],j,\mathbf{k}[1]} \otimes \tilde{\psi}_{\mathbf{s}[2],j,\mathbf{k}[2]} \otimes \tilde{\psi}_{\mathbf{s}[3],j,\mathbf{k}[3]}, \quad (18)$$

where  $j \in \mathbb{Z}$ ,  $\mathbf{k} \in \mathbb{Z}^3$ , and  $\mathbf{s} \in \{0,1\}^3$ . Now an arbitrary function in the space where the MRA is constructed can be represented as

$$f(\mathbf{x}) = \sum_{\mathbf{k} \in \mathbb{Z}^3} c_{j_{\min},\mathbf{k}} \varphi_{j_{\min},\mathbf{k}}(\mathbf{x}) + \sum_{j=j_{\min}}^{\infty} \sum_{\mathbf{s} \in J_+} \sum_{\mathbf{k} \in \mathbb{Z}^3} d_{\mathbf{s},j,\mathbf{k}} \psi_{\mathbf{s},j,\mathbf{k}}(\mathbf{x}) \quad (19)$$

where  $c_{j_{\min},\mathbf{k}} = \langle \tilde{\varphi}_{j_{\min},\mathbf{k}}, f \rangle$ ,  $d_{\mathbf{s},j,\mathbf{k}} = \langle \tilde{\psi}_{\mathbf{s},j,\mathbf{k}}, f \rangle$ , and  $J_+ = \{0,1\}^3 \setminus \{0,0,0\}$ .

There is an alternative way to index the multi-dimensional basis functions in a three-dimensional point grid. In this formulation the index is a point located at the “peak” of the basis function (for the mother scaling function this peak is located at the origin).

Define

$$Z_j = \left\{ \frac{k}{2^j} \mid k \in \mathbb{Z} \right\} \quad (20)$$

and

$$V_j = Z_j^3 \quad (21)$$

where  $j \in \mathbb{Z}$ . Define sets  $Q_j$  by

$$Q_{j_{\min}} = V_{j_{\min}} \quad (22)$$

$$Q_j = V_j \setminus V_{j-1} \text{ for } j > j_{\min} \quad (23)$$

The point grid  $G$  shall be some finite subset of  $V_{j_{\max}}$ . We use only bases with one or two resolution levels  $j$  in this article. We define

$$G_j := G \cap Q_j \quad (24)$$

for  $j \geq j_{\min}$ .

Define

$$\eta_{j,k} := \begin{cases} \varphi_{j_{\min},k}; & \text{if } j = j_{\min} \\ \varphi_{j-1,k/2}; & \text{if } j > j_{\min} \text{ and } k \text{ even} \\ \psi_{j-1,(k-1)/2}; & \text{if } j > j_{\min} \text{ and } k \text{ odd} \end{cases} \quad (25)$$

$$\tilde{\eta}_{j,k} := \begin{cases} \tilde{\varphi}_{j_{\min},k}; & \text{if } j = j_{\min} \\ \tilde{\varphi}_{j-1,k/2}; & \text{if } j > j_{\min} \text{ and } k \text{ even} \\ \tilde{\psi}_{j-1,(k-1)/2}; & \text{if } j > j_{\min} \text{ and } k \text{ odd} \end{cases} \quad (26)$$

When  $\alpha \in Q_j$  and  $j \geq j_{\min}$  define

$$\zeta_{\alpha} := \eta_{j,\mathbf{k}[1]} \otimes \eta_{j,\mathbf{k}[2]} \otimes \eta_{j,\mathbf{k}[3]} \quad (27)$$

and

$$\tilde{\zeta}_{\alpha} := \tilde{\eta}_{j,\mathbf{k}[1]} \otimes \tilde{\eta}_{j,\mathbf{k}[2]} \otimes \tilde{\eta}_{j,\mathbf{k}[3]} \quad (28)$$

where  $\mathbf{k} = 2^j \alpha$ .

One-dimensional case is similar. We set  $Q_j = Z_j$  and  $\zeta_{\alpha} = \eta_{j,k}$ ,  $\tilde{\zeta}_{\alpha} = \tilde{\eta}_{j,k}$  for  $k = 2^j \alpha$ .

### 3.2 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

$$\zeta_{j,k} = \begin{cases} \varphi_{j_{\min},k} = 2^{j/2} \varphi(2^j \cdot -k) & j = j_{\min} \\ \psi_{j-1,k} = 2^{(j-1)/2} \psi(2^{j-1} \cdot -k) & j > j_{\min} \end{cases} \quad (29)$$

where  $(j, k) \in I$ ,  $\varphi$  is the mother scaling function of the wavelet family, and  $\psi$  is the mother wavelet of the wavelet family.

We have

$$\varphi(x) = \sum_{k=0}^{M-1} a_k \varphi(2x - k), \quad (30)$$

$$\psi(x) = \sum_{k=0}^{M-1} b_k \varphi(2x - k), \quad (31)$$

where  $M$  is a positive integer,  $a_k$  are real numbers, and  $b_k = (-1)^k a_{M-1-k}$ .

An arbitrary function  $f \in L^2(\mathbb{R})$  can be represented as

$$f(x) = \sum_k c_{j_{\min},k} \varphi_{j_{\min},k}(x) + \sum_{j=j_{\min}}^{\infty} \sum_k d_{j,k} \psi_{j,k}(x) \quad (32)$$

where

$$c_{j_{\min},k} = \int_{\mathbb{R}} \varphi_{j_{\min},k}(x) f(x) dx \quad (33)$$

and

$$d_{j,k} = \int_{\mathbb{R}} \psi_{j,k}(x) f(x) dx. \quad (34)$$

## 4 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. [17].

A stationary state  $\psi$  of a quantum mechanical system can be represented by

$$\chi(\mathbf{x}) = \sum_{k=0}^{\infty} c_k \chi_k(\mathbf{x}) \quad (35)$$

where functions  $\chi_k$  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

$$\Psi(\mathbf{x}, t) = \sum_{k=0}^{\infty} c_k \exp(-iE_k t) \chi_k(\mathbf{x}) \quad (36)$$

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

$$\hat{g}(\omega) = \frac{1}{\sqrt{2\pi}} \int_{t=-\infty}^{\infty} g(t) \exp(-i\omega t) dt \quad (37)$$

$$= \frac{1}{\sqrt{2\pi}} \sum_{k=0}^{\infty} c_k \chi_k(\mathbf{x}_0) \int_{t=-\infty}^{\infty} \exp(-iE_k t) \exp(-i\omega t) dt \quad (38)$$

$$= \sqrt{2\pi} \sum_{k=0}^{\infty} c_k \chi_k(\mathbf{x}_0) \delta(\omega + E_k). \quad (39)$$

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  $\chi_i(\mathbf{x}) = \Psi(\mathbf{x}, t_i)$  and final state  $\chi_f(\mathbf{x}) = \Psi(\mathbf{x}, t_f)$  and assume that the time interval  $\Delta t := t_b - t_a$  is small. We have

$$\chi_f(\mathbf{x}) - \chi_i(\mathbf{x}) = (\exp(-iEt) - 1) \chi_i(\mathbf{x}) \approx -iEt \chi_i(\mathbf{x}) \quad (40)$$

from which we obtain

$$E \approx -\frac{1}{\Delta t} \text{Im} \frac{\chi_f(\mathbf{x}) - \chi_i(\mathbf{x})}{\chi_i(\mathbf{x})} \quad (41)$$

and

$$\langle E \rangle \approx -\frac{1}{\Delta t} \text{Im} \int_{\mathbb{R}^d} (\chi_f(\mathbf{x}) - \chi_i(\mathbf{x})) (\chi_i(\mathbf{x}))^* d\mathbf{x}. \quad (42)$$

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 function  $-\varphi_{j_{\min}, -1} + \varphi_{j_{\min}, 1}$  is used instead of the derivative. In three dimensions the tensor products of functions  $(-1 - i)\varphi_{j_{\min}, -1} + (1 + i)\varphi_{j_{\min}, 0} + (1 + i)\varphi_{j_{\min}, 1}$  are used.

The continuous Fourier transform is computed by the method described in [18, section 2]. We have also generalized it into three dimensions.

Let  $\mathbf{x}_j, j = 1, \dots, N$  be the points where the wavefunction of state  $k$  shall be calculated. Let  $g_j(t) := \Psi(\mathbf{x}_j, t)$  and  $\Delta E$  be the spacing between points in the Fourier spectrum  $\hat{g}_j(E)$ . We approximate the Dirac  $\delta$  functions in equation (39) with a Gaussian function and we assume that the overlaps of the approximated peaks can be neglected. The square of each Gaussian peak is another Gaussian peak and the peak  $k$  is fitted to the Gaussian distribution

$$G_{k,j}(E) = \frac{1}{\sigma_{k,j} \sqrt{2\pi}} \exp\left(-\frac{(E + E_k)^2}{2\sigma_{k,j}^2}\right) \quad (43)$$

using the computed values of  $|\hat{g}_j(E)|^2$ . Define

$$p_{k,j} = |\hat{g}_j(-E_k)|^2 \quad (44)$$

and

$$p'_{k,j} = \frac{1}{2} \left( |\hat{g}_j(-E_k + \Delta E)|^2 + |\hat{g}_j(-E_k - \Delta E)|^2 \right). \quad (45)$$

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

$$p_{k,j} = d_{k,j} G_{k,j}(-E_k) = d_{k,j} \frac{1}{\sqrt{2\pi}} \frac{1}{\sigma_{k,j}} \quad (46)$$

and

$$p'_{k,j} = d_{k,j} G_{k,j}(-E_k + \Delta E) = d_{k,j} \frac{1}{\sqrt{2\pi}} \frac{1}{\sigma_{k,j}} \exp\left(-\frac{\Delta E^2}{2\sigma_{k,j}^2}\right) \quad (47)$$

It follows that

$$d_{k,j} = \sqrt{2\pi} \sigma_{k,j} p_{k,j} \quad (48)$$

and

$$\sigma_{k,j} = \Delta E / \sqrt{2 \ln \frac{p_{k,j}}{p'_{k,j}}}. \quad (49)$$

The FWHM (full width at half maximum)  $\Gamma_{k,j}$  of the peak  $k$  computed at point  $\mathbf{x}_j$  determines quantity  $\sigma_{k,j}$  [19]:

$$\sigma_{k,j} = \frac{1}{2\sqrt{2 \ln 2}} \Gamma_{k,j}. \quad (50)$$

The product of the height of a peak and its FWHM determines the probability density of eigenstate  $\chi_k$  at the point  $\mathbf{x}_j$  where the spectrum is computed, see formulas (48) and (50).

## 5 Approximation of the Path Integral Kernel

We assume that the potential  $V$  is time-independent. The kernel is approximated by setting  $N = 2$ . Thus

$$K_2(\mathbf{x}_b, \mathbf{x}_a; \epsilon) := \left(\frac{m}{2\pi i \epsilon}\right)^d \int_{\mathbb{R}^d} \exp(iS_2) d\mathbf{x}_1. \quad (51)$$

We have

$$K_2(\mathbf{x}_b, \mathbf{x}_a; \epsilon) = \left(\frac{m}{2\pi i \epsilon}\right)^d I \quad (52)$$

where

$$I := \int_{\mathbf{x}_1 \in \mathbb{R}^d} \exp(iS_2) d\mathbf{x}_1 \quad (53)$$

$$\begin{aligned} &= \int_{\mathbf{x}_1 \in \mathbb{R}^d} \exp\left(i\epsilon \left(\frac{m}{2} \left(\frac{\mathbf{x}_1 - \mathbf{x}_a}{\epsilon}\right)^2 - V(\mathbf{x}_1) + \frac{m}{2} \left(\frac{\mathbf{x}_b - \mathbf{x}_1}{\epsilon}\right)^2 - V(\mathbf{x}_b)\right)\right) d\mathbf{x}_1 \quad (54) \end{aligned}$$

$$\begin{aligned} &= \exp\left(i\left(\frac{m}{2\epsilon} (\mathbf{x}_b^2 + \mathbf{x}_a^2) - \epsilon V(\mathbf{x}_b)\right)\right) \int_{\mathbf{x}_1 \in \mathbb{R}^d} \exp\left(i\left(\frac{m}{\epsilon} \mathbf{x}_1^2 - \epsilon V(\mathbf{x}_1)\right)\right) \exp\left(-i\frac{m}{\epsilon} (\mathbf{x}_b + \mathbf{x}_a) \cdot \mathbf{x}_1\right) d\mathbf{x}_1 \quad (55) \end{aligned}$$

$$= \sqrt{2\pi}^{-d} \exp\left(i\left(\frac{m}{2\epsilon} (\mathbf{x}_b^2 + \mathbf{x}_a^2) - \epsilon V(\mathbf{x}_b)\right)\right) \hat{h}\left(\frac{m}{\epsilon} (\mathbf{x}_b + \mathbf{x}_a)\right) \quad (56)$$

and

$$h(\mathbf{x}_1) := \exp\left(i\left(\frac{m}{\epsilon}\mathbf{x}_1^2 - \epsilon V(\mathbf{x}_1)\right)\right). \quad (57)$$

Now

$$K_2(\mathbf{x}_b, \mathbf{x}_a; \epsilon) = \left(\frac{m}{2\pi i \epsilon} \sqrt{2\pi}\right)^d \exp\left(i\left(\frac{m}{2\epsilon}(\mathbf{x}_b^2 + \mathbf{x}_a^2) - \epsilon V(\mathbf{x}_b)\right)\right) \hat{h}\left(\frac{m}{\epsilon}(\mathbf{x}_b + \mathbf{x}_a)\right). \quad (58)$$

We call this kernel the *midpoint kernel*.

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

$$\hat{h}(\mathbf{k}) = \frac{i}{2k} \left( \hat{f}(k) - \hat{f}(-k) \right), \quad (59)$$

where  $f(r) = r h_{\text{rad}}(|r|)$  and  $h(\mathbf{r}) = h_{\text{rad}}(|\mathbf{r}|)$ . Note that the Fourier transform of  $f$  in equation (59) is one-dimensional. See Ref. [1, section 3-11] for another Fourier transform based approach to the path integral formulation.

## 6 Quantum Harmonic Oscillator and Hydrogen-like Atom

The potential of the one-dimensional harmonic oscillator is

$$V(x) = \frac{m\omega_0^2}{2}x^2 \quad (60)$$

where  $m$  is the mass of the particle and  $\omega_0$  is the angular frequency. The potential of the isotropic three-dimensional harmonic oscillator is

$$V(\mathbf{x}) = \frac{m\omega_0^2}{2}|\mathbf{x}|^2. \quad (61)$$

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

$$K(x_b, x_a; t) = \left(\frac{m\omega_0}{2\pi i \sin(\omega_0 t)}\right)^{1/2} \exp(iS_{\text{cl}}), \quad (62)$$

where  $S_{\text{cl}}$  is the classical action given by

$$S_{\text{cl}} = \frac{m\omega_0}{2\sin(\omega_0 t)} \left( (x_b^2 + x_a^2) \cos(\omega_0 t) - 2x_b x_a \right). \quad (63)$$

By substituting the potential of the one-dimensional harmonic oscillator to equation (57) we obtain

$$h(x_1) = \exp\left(i\frac{m}{\epsilon}\left(1 - \frac{\epsilon^2\omega_0^2}{2}\right)x_1^2\right). \quad (64)$$

Define

$$c := \frac{m}{\epsilon}\left(1 - \frac{\epsilon^2\omega_0^2}{2}\right) \quad (65)$$



and assume that  $c > 0$ . Now

$$\hat{h}(k) = \frac{1}{2}(1 + i)\frac{1}{\sqrt{c}}\exp\left(-i\frac{k^2}{4c}\right). \quad (66)$$

Similarly, in the three-dimensional case we have

$$\hat{h}(\mathbf{k}) = \frac{1}{4}(-1 + i)c^{-3/2}\exp\left(-i\frac{k^2}{4c}\right) \quad (67)$$

using equation (59).

The potential of a hydrogen-like atom is

$$V(x) = -\frac{Z}{|x|} \quad (68)$$

in one dimension and

$$V(\mathbf{x}) = -\frac{Z}{|\mathbf{x}|} \quad (69)$$

in three dimensions. Here  $Z$  is the atomic number. The Trotter kernel for a hydrogen-like atom is computed by equation (9) and the midpoint kernel by equation (58).

## 7 Representation of the Path-Integral Kernel in Wavelet Bases

### 7.1 Interpolating Wavelets

The interpolating mother scaling function can be represented as [7, 9]

$$\varphi(x) = \sum_{\alpha \in \mathbb{Z}} s[\alpha]\varphi(2^J x - \alpha) \quad (70)$$

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

$$\eta_{j_{\min}, k}(2^{-J-j_{\min}}p) = s_0[p - 2^J k] \quad (71)$$

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

$$\eta_{j_{\min}+1, k}(2^{-J-j_{\min}}p) = s_0[p - 2^{J-1}k] \quad (72)$$

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

$$\eta_{j_{\min}+1, k}(2^{-J-j_{\min}}p) = s_1[p - 2^{J-1}k] \quad (73)$$

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

$$\tilde{\eta}_{j_{\min}, \ell} = \tilde{\varphi}_{j_{\min}, \ell} = \delta(\cdot - 2^{-j_{\min}}\ell) \quad (74)$$

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

$$\tilde{\eta}_{j_{\min}+1, \ell} = \delta(\cdot - 2^{-j_{\min}-1}\ell) = \sum_{\beta \in \mathbb{Z}} \tilde{h}_{\beta}\delta(\cdot - 2^{-j_{\min}-1}(\beta + \ell)) \quad (75)$$

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

$$\tilde{\eta}_{j_{\min}+1,\ell} = \sum_{\beta \in \mathbb{Z}} \tilde{g}_{\beta} \delta(\cdot - 2^{-j_{\min}-1}(\beta + \ell - 1)) \quad (76)$$

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

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

$$K_{\mathbf{r},\mathbf{q}} = \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \tilde{\zeta}_{\mathbf{r}}(\mathbf{y}) K(\mathbf{y}, \mathbf{x}; \epsilon) \zeta_{\mathbf{q}}(\mathbf{x}) d\mathbf{x} d\mathbf{y}. \quad (77)$$

It follows from equation (11) that the dual wavelets  $\tilde{\zeta}_{\mathbf{r}}$  are finite sums of delta distributions. Consequently the integration over  $\mathbf{y}$  is actually a weighted sum of values of the function

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

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

$$K_{\mathbf{r},\mathbf{q}} = \int_{\mathbb{R}^d} K(2^{-j_{\min}} \ell, \mathbf{x}; \epsilon) \zeta_{\mathbf{q}}(\mathbf{x}) d\mathbf{x}. \quad (78)$$

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

$$\int_{\mathbb{R}} K(y, x; \epsilon) \zeta_q(x) dx \approx 2^{-j_{\min}-J} \sum_{p \in \mathbb{Z}} K(y, 2^{-j_{\min}-J} p; \epsilon) s_{t(q)}(p - 2^{J-t(q)} k) \quad (79)$$

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

$$t(q) := \begin{cases} 1 & \text{if } q \in G_{j_{\min}+1} \\ 0 & \text{if } q \in G_{j_{\min}}. \end{cases} \quad (80)$$

For the three-dimensional case define

$$T(\mathbf{q}) := \begin{cases} 1 & \text{if } \mathbf{q} \in G_{j_{\min}+1} \\ 0 & \text{if } \mathbf{q} \in G_{j_{\min}} \end{cases} \quad (81)$$

and

$$t_i(\mathbf{q}) := \begin{cases} 1 & \text{if } \mathbf{q} \in G_{j_{\min}+1} \text{ and } 2^{j_{\min}+1} \mathbf{q}[i] \text{ odd} \\ 0 & \text{otherwise} \end{cases} \quad (82)$$

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

$$s_{\mathbf{t}}[\mathbf{z}] := s_{t[1]}[\mathbf{z}[1]] s_{t[2]}[\mathbf{z}[2]] s_{t[3]}[\mathbf{z}[3]]. \quad (83)$$

Now we can approximate

$$\int_{\mathbb{R}^3} K(\mathbf{y}, \mathbf{x}; \epsilon) \zeta_{\mathbf{q}}(\mathbf{x}) d\mathbf{x} \approx 2^{-3(j_{\min}+J)} \sum_{\mathbf{p} \in \mathbb{Z}^3} K(\mathbf{y}, 2^{-j_{\min}-J} \mathbf{p}; \epsilon) s_{\mathbf{t}(\mathbf{q})}[\mathbf{p} - 2^{J-T(\mathbf{q})} \mathbf{k}] \quad (84)$$

where  $\mathbf{k} \in \mathbb{Z}^3$  and  $\mathbf{q} = 2^{-j_{\min}} \mathbf{k} \in G_{j_{\min}}$  or  $\mathbf{q} = 2^{-j_{\min}-1} \mathbf{k} \in G_{j_{\min}+1}$ . 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 (70) 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.

## 7.2 Orthonormal Wavelets

In order to compute the values of the orthonormal wavelets we use the representation

$$\varphi(x) = 2^{J/2} \sum_{\alpha \in \mathbb{Z}} w[\alpha] \varphi(2^J x - \alpha) \quad (85)$$

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

$$K_{j,k,j',k'} = \int_{\mathbb{R}} \int_{\mathbb{R}} \zeta_{j,k}(y) K(y, x; \epsilon) \zeta_{j',k'}(x) dx dy \quad (86)$$

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

## 8 Test Results

Unless otherwise stated the calculations use Deslauriers–Dubuc wavelets. The vertical axes of the energy spectra contain quantity  $|G(E)|$ , where  $G(E)$  is an approximation of function  $\hat{g}(-E)$  and function  $g$  is defined in section 4. The notation of the spectra is the following:

- The locations of the peaks determine the energy eigenstates of the system.
- The heights and widths of the peaks determine the values of the probability densities at the points where the spectra are computed.

The construction of the basis sets has been presented in section 3. For Deslauriers–Dubuc wavelets, the notation for the point grid  $G$  is

$$G = 2^{-j_{\min}} \{k_{\min}^0, \dots, k_{\max}^0\}^d \quad (87)$$

or

$$G = 2^{-j_{\min}} \{k_{\min}^0, \dots, k_{\max}^0\}^d \cup 2^{-j_{\min}-1} \{k_{\min}^1, \dots, k_{\max}^1\}^d \quad (88)$$

where  $d$  is the dimensionality of the system,  $d = 1$  or  $d = 3$ . For Daubechies wavelets, the notation for the basis set is

$$I = \{(j_{\min}, k) : k = k_{\min}^0, \dots, k_{\max}^0\} \quad (89)$$

or

$$I = \{(j_{\min}, k) : k = k_{\min}^0, \dots, k_{\max}^0\} \cup \{(j_{\min} + 1, k) : k = k_{\min}^1, \dots, k_{\max}^1\}. \quad (90)$$

The time step  $\Delta t = t_b - t_a$  has been defined by equations (6), (7), and (8). The scaling function resolution  $J$  has been defined in section 7.

## 8.1 Harmonic Oscillator

The one-dimensional harmonic oscillator is calculated 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. The basis  $(1/4)\{-48, \dots, 48\}$  is used for one-level calculations and the basis  $(1/4)\{-48, \dots, 48\} \cup (1/8)\{-5, \dots, 5\}$  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 4 is plotted in Fig. 3.

The three-dimensional harmonic oscillator is calculated 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  $\{-10, \dots, 10\}^3$  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. 4. 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..

## 8.2 Hydrogen Atom

When the Deslauriers–Dubuc (interpolating) wavelets are used for the hydrogen atom the midpoint kernel 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 the basis  $\{(2, -48), \dots, (2, 48)\}$  is used and for the two-level calculations the basis  $\{(1, -24), \dots, (1, 24)\} \cup \{(2, -6), \dots, (2, 6)\}$ . We set the mother scaling function resolution to  $J = 5$ . The resulting ground state energies and first excited state energies are presented in figures 5 and 6. 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 than 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. As regards the first excited state, the best energy for the Trotter kernel is  $E_1 = -0.125664$  Ha and for the midpoint kernel  $E_1 = -0.119381$  Ha.

The best energy spectrum for the Trotter kernel is plotted in Fig. 7 and for the midpoint kernel in Fig. 8. The radial probability density function of the hydrogen atom calculated in one dimension with the the method described in section 4 is plotted in Fig. 9.

We make three-dimensional calculations of the hydrogen atom using the midpoint kernel and the Trotter kernel. The basis function set is  $(1/2)\{-9, \dots, 9\}^3 \cup (1/4)\{-4, \dots, 4\}^3$ . The function  $\hat{h}(\mathbf{k})$  for the midpoint kernel is calculated with formula (59). The sign of the midpoint kernel (58) has to be inverted in order to

get the energy computation to work. We get energy  $E = -0.537212$  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  $E = -0.471239$  Ha with parameter  $\Delta t = 0.2$  a.u. and value  $\Delta t = 0.125$  a.u. does not give reasonable results.

## 9 Conclusions

The new issues in this article are:

- Use of Deslauriers–Dubuc and Daubechies wavelets with the path integral formulation
- The midpoint kernel approximation of the path integral kernel
- A method to compute probability density of a quantum state with the path integral formulation

We estimate the goodness of the test results by comparing the energy eigenvalues to the exact energies of the test systems and comparing the computed probability density curves to the exact ones. The relative errors of the computed energies were:

- Ground state and first excited state of the one-dimensional harmonic oscillator: 0.5%
- Ground state and first excited state of the three-dimensional harmonic oscillator: 0.5%
- Hydrogen atom ground state computed with one dimension and the midpoint kernel: 0.7%
- Hydrogen atom first excited state computed with one dimension and the midpoint kernel: 4%
- Hydrogen atom ground state computed with three dimensions and the midpoint kernel: 7%

These results are good except the last two ones. However, these energies are reasonable approximations. Our algorithm gave good results for the probability density functions: the computed and exact curves were almost the same. Both the Deslauriers–Dubuc wavelets and Daubechies wavelets were useful basis sets for the computations. It turned out that when the time step parameter  $\Delta t$  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  $\Delta t$ . The two kernels yield approximately the same energy for the harmonic oscillator.

Note that many different calculations yield exactly same energy values because the energy spectrum  $\hat{g}(-E)$  is approximated by the Discrete Fourier Transform, for which the energy values are discrete. Ruokosenmäki [16] has discussed the behavior of the path integral kernel with small values of  $\Delta t$ , too.

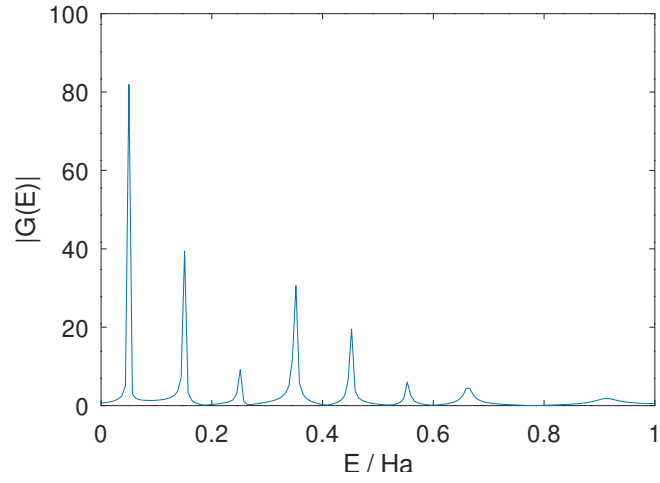


Figure 1: Energy spectrum of the one-dimensional harmonic oscillator computed with the exact kernel.

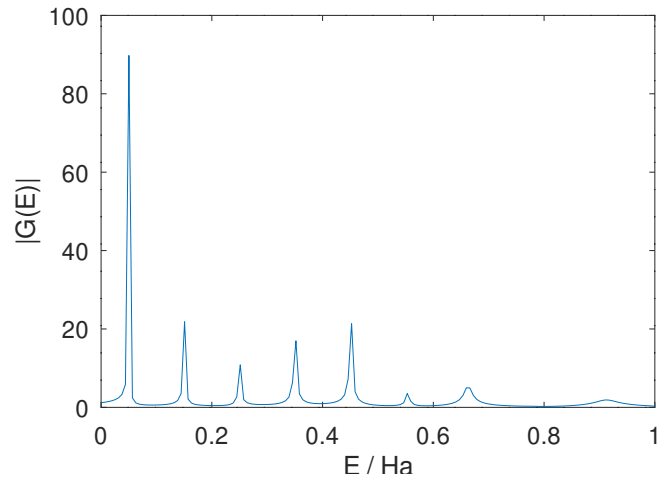


Figure 2: Energy spectrum of the one-dimensional harmonic oscillator computed with the midpoint kernel.

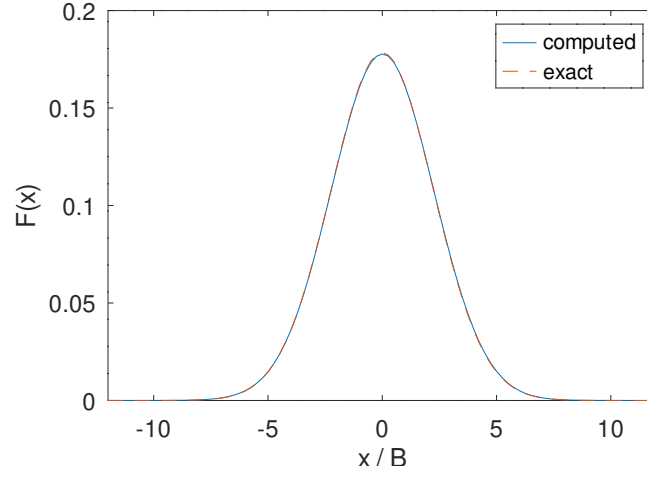


Figure 3: Probability density function  $F(x) = |\psi(x)|^2$  of the one-dimensional harmonic oscillator computed with the exact kernel.

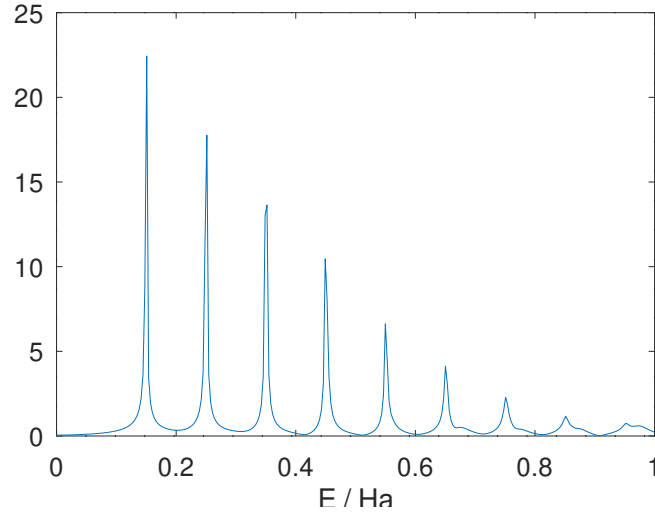


Figure 4: Energy spectrum of the three-dimensional harmonic oscillator calculated with the midpoint kernel.

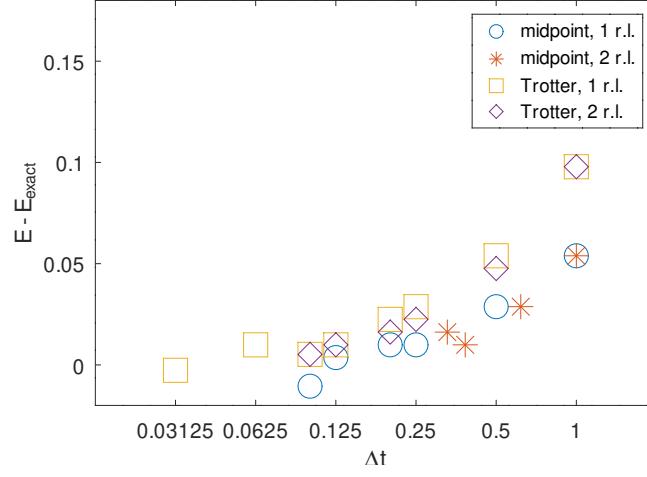


Figure 5: Energies of the hydrogen atom ground state. “Midpoint” and “Trotter” denote the kernel type and “r.l.” stands for number of resolution levels.

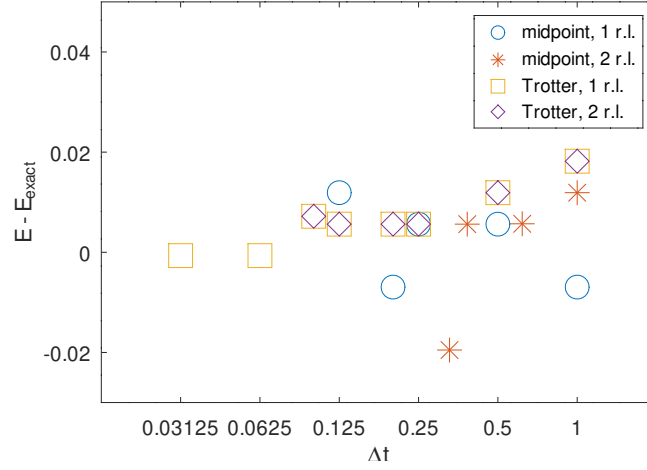


Figure 6: Energies of the first excited state of the hydrogen atom. “Midpoint” and “Trotter” denote the kernel type and “r.l.” stands for number of resolution levels.



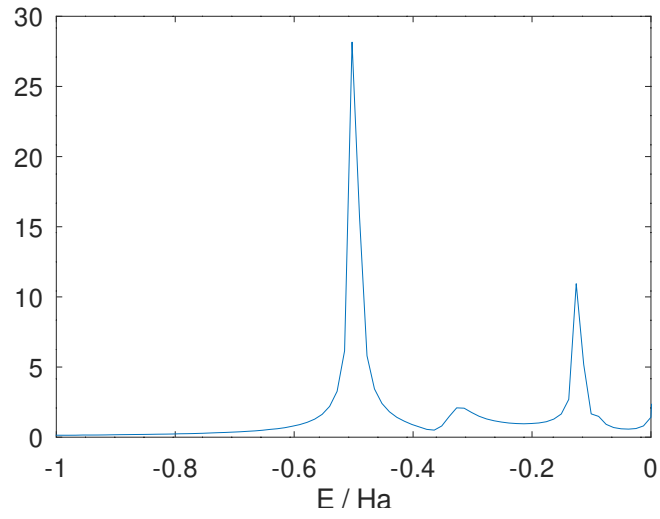


Figure 7: Energy spectrum of the hydrogen atom computed with the Trotter kernel in one dimension.

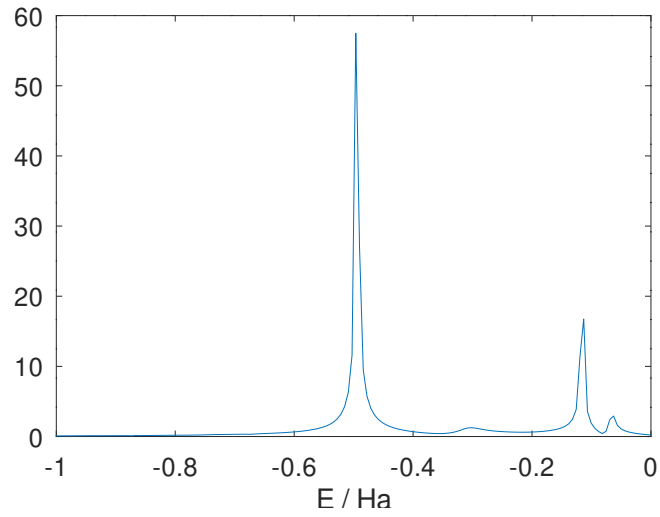


Figure 8: Energy spectrum of the hydrogen atom computed with the midpoint kernel in one dimension.

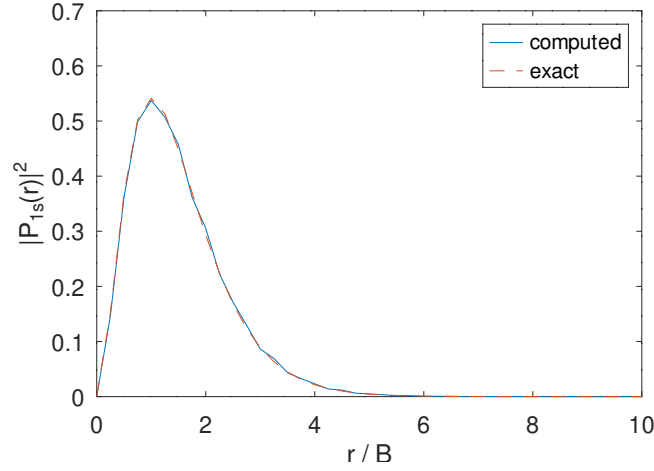


Figure 9: Radial probability density function  $|P_{1s}(r)|^2$  of the hydrogen atom computed with the midpoint kernel in one dimension.

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