

Fourier transform and wavelet approaches to the path integral formulation

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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

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

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

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

$L(\mathbf{x}(t), \dot{\mathbf{x}}(t))$ is the Lagrangian of the system, and ψ_0 is the initial state. See Ref. [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.

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[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 ($e = m_e = \hbar = 4\pi\epsilon_0 = 1$) 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. We denote a stationary wavefunction by χ as the symbol ψ is used for wavelets. 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

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2 Path Integral Formulation

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

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

For a stationary system it 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 is given by

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

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]

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

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

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

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

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

and

$$\epsilon = \frac{t_b - t_a}{N}. \quad (9)$$

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

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

3 Wavelet Bases

3.1 Interpolating Wavelets

We construct the basis function set in the same way as in Ref. [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 . 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 φ satisfies the relation

$$\varphi(x) = \sum_{\mu} h_{\mu} \varphi(2x - \mu) \quad (11)$$

and the mother wavelet is given by $\psi(x) = \varphi(2x - 1)$. We assume that the filter h_{μ} 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

$$\tilde{\psi} = 2 \sum_{\nu} \tilde{g}_{\nu} \delta(2 \cdot - \nu) \quad (12)$$

and $\tilde{g}_{\nu} = (-1)^{\nu-1} h_{1-\nu}$. When we construct an interpolating wavelet basis 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

$$f(x) = \sum_k c_{j_{\min},k} \varphi_{j_{\min},k}(x) + \sum_{j=j_{\min}}^{\infty} \sum_k d_{j,k} \psi_{j,k}(x) \quad (13)$$

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

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

and

$$\tilde{\psi}_{s,j,k} = \begin{cases} \varphi_{j,k}; & \text{if } s = 0 \\ \psi_{j,k}; & \text{if } s = 1 \end{cases} \quad (15)$$

For the three-dimensional case we define

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

$$\psi_{\mathbf{s},j,\mathbf{k}}(\mathbf{x}) = \psi_{\mathbf{s}[1],j,\mathbf{k}[1]}(\mathbf{x}[1])\psi_{\mathbf{s}[2],j,\mathbf{k}[2]}(\mathbf{x}[2])\psi_{\mathbf{s}[3],j,\mathbf{k}[3]}(\mathbf{x}[3]), \quad (17)$$

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

$$\tilde{\psi}_{\mathbf{s},j,\mathbf{k}} = \tilde{\psi}_{\mathbf{s}[1],j,\mathbf{k}[1]} \otimes \tilde{\psi}_{\mathbf{s}[2],j,\mathbf{k}[2]} \otimes \tilde{\psi}_{\mathbf{s}[3],j,\mathbf{k}[3]}, \quad (19)$$

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

$$f(\mathbf{x}) = \sum_{\mathbf{k} \in \mathbb{Z}^3} c_{j_{\min},\mathbf{k}} \varphi_{j_{\min},\mathbf{k}}(\mathbf{x}) + \sum_{j=j_{\min}}^{\infty} \sum_{\mathbf{s} \in J_+} \sum_{\mathbf{k} \in \mathbb{Z}^3} d_{\mathbf{s},j,\mathbf{k}} \psi_{\mathbf{s},j,\mathbf{k}}(\mathbf{x}) \quad (20)$$

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

$$Z_j = \left\{ \frac{k}{2^j} \mid k \in \mathbb{Z} \right\} \quad (21)$$

and

$$V_j = Z_j^3 \quad (22)$$

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

$$Q_{j_{\min}} = V_{j_{\min}} \quad (23)$$

$$Q_j = V_j \setminus V_{j-1} \text{ for } j > j_{\min} \quad (24)$$

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

$$G_j := G \cap Q_j \quad (25)$$

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

$$\eta_{j,k} := \begin{cases} \varphi_{j_{\min},k}; & \text{if } j = j_{\min} \\ \varphi_{j-1,k/2}; & \text{if } j > j_{\min} \text{ and } k \text{ even} \\ \psi_{j-1,(k-1)/2}; & \text{if } j > j_{\min} \text{ and } k \text{ odd} \end{cases} \quad (26)$$

$$\tilde{\eta}_{j,k} := \begin{cases} \tilde{\varphi}_{j_{\min},k}; & \text{if } j = j_{\min} \\ \tilde{\varphi}_{j-1,k/2}; & \text{if } j > j_{\min} \text{ and } k \text{ even} \\ \tilde{\psi}_{j-1,(k-1)/2}; & \text{if } j > j_{\min} \text{ and } k \text{ odd} \end{cases} \quad (27)$$

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

$$\zeta_\alpha := \eta_{j,\mathbf{k}[1]} \otimes \eta_{j,\mathbf{k}[2]} \otimes \eta_{j,\mathbf{k}[3]} \quad (28)$$

and

$$\tilde{\zeta}_\alpha := \tilde{\eta}_{j,\mathbf{k}[1]} \otimes \tilde{\eta}_{j,\mathbf{k}[2]} \otimes \tilde{\eta}_{j,\mathbf{k}[3]} \quad (29)$$

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

3.2 Orthonormal Wavelets

See Ref. [18] 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

$$\zeta_{j,k} = \begin{cases} \varphi_{j_{\min},k} = 2^{j/2} \varphi(2^j \cdot -k) & j = j_{\min} \\ \psi_{j-1,k} = 2^{(j-1)/2} \psi(2^{j-1} \cdot -k) & j > j_{\min} \end{cases} \quad (30)$$

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.

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. [5].

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

$$\chi(\mathbf{x}) = \sum_{k=0}^{\infty} c_k \chi_k(\mathbf{x}) \quad (31)$$

where functions χ_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

$$\Psi(\mathbf{x}, t) = \sum_{k=0}^{\infty} c_k \exp(-iE_k t) \chi_k(\mathbf{x}) \quad (32)$$

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

$$\hat{g}(\omega) = \frac{1}{\sqrt{2\pi}} \int_{t=-\infty}^{\infty} g(t) \exp(-i\omega t) dt \quad (33)$$

$$= \frac{1}{\sqrt{2\pi}} \sum_{k=0}^{\infty} c_k \chi_k(\mathbf{x}_0) \int_{t=-\infty}^{\infty} \exp(-iE_k t) \exp(-i\omega t) dt \quad (34)$$

$$= \sqrt{2\pi} \sum_{k=0}^{\infty} c_k \chi_k(\mathbf{x}_0) \delta(\omega + E_k). \quad (35)$$

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

$$\chi_f(\mathbf{x}) - \chi_i(\mathbf{x}) = (\exp(-iEt) - 1) \chi_i(\mathbf{x}) \approx -iEt\chi_i(\mathbf{x}) \quad (36)$$

from which we obtain

$$E \approx -\frac{1}{\Delta t} \text{Im} \frac{\chi_f(\mathbf{x}) - \chi_i(\mathbf{x})}{\chi_i(\mathbf{x})} \quad (37)$$

and

$$\langle E \rangle \approx -\frac{1}{\Delta t} \text{Im} \int_{\mathbb{R}^d} (\chi_f(\mathbf{x}) - \chi_i(\mathbf{x})) (\chi_i(\mathbf{x}))^* d\mathbf{x}. \quad (38)$$

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 $(-1-i)\varphi_{j_{\min},-1} + (1+i)\varphi_{j_{\min},0} + (1+i)\varphi_{j_{\min},1}$.

We use the method described in [19, section 2] to compute the continuous Fourier transform. We have also generalized it into three dimensions.

Let \mathbf{x}_j , $j = 1, \dots, N$ 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 approximate the Dirac δ functions in equation (35) 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 we fit the peak k to the Gaussian distribution

$$G_{k,j}(E) = \frac{1}{\sigma_{k,j} \sqrt{2\pi}} \exp\left(-\frac{(E + E_k)^2}{2\sigma_{k,j}^2}\right) \quad (39)$$

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

$$p_{k,j} = |\hat{g}_j(-E_k)|^2 \quad (40)$$

and

$$p'_{k,j} = \frac{1}{2} \left(|\hat{g}_j(-E_k + \Delta E)|^2 + |\hat{g}_j(-E_k - \Delta E)|^2 \right). \quad (41)$$

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

$$p_{k,j} = d_{k,j} G_{k,j}(-E_k) = d_{k,j} \frac{1}{2\pi} \frac{1}{\sigma_{k,j}} \quad (42)$$

and

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

It follows that

$$d_{k,j} = \sqrt{2\pi} \sigma_{k,j} p_{k,j} \quad (44)$$

and

$$\sigma_{k,j} = \Delta E / \sqrt{2 \ln \frac{p_{k,j}}{p'_{k,j}}}. \quad (45)$$

5 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

$$K_2(\mathbf{x}_b, \mathbf{x}_a; \epsilon) := \left(\frac{m}{2\pi i \epsilon}\right)^d \int_{\mathbb{R}^d} \exp(iS_2) d\mathbf{x}_1. \quad (46)$$

We have

$$K_2(\mathbf{x}_b, \mathbf{x}_a; \epsilon) = \left(\frac{m}{2\pi i \epsilon}\right)^d I \quad (47)$$

where

$$I := \int_{\mathbf{x}_1 \in \mathbb{R}^d} \exp(iS_2) d\mathbf{x}_1 \quad (48)$$

$$= \int_{\mathbf{x}_1 \in \mathbb{R}^d} \exp\left(i\epsilon \left(\frac{m}{2} \left(\frac{\mathbf{x}_1 - \mathbf{x}_a}{\epsilon}\right)^2 - V(\mathbf{x}_1) + \frac{m}{2} \left(\frac{\mathbf{x}_b - \mathbf{x}_1}{\epsilon}\right)^2 - V(\mathbf{x}_b)\right)\right) d\mathbf{x}_1 \quad (49)$$

$$= \exp\left(i\left(\frac{m}{2\epsilon}(\mathbf{x}_b^2 + \mathbf{x}_a^2) - \epsilon V(\mathbf{x}_b)\right)\right) \int_{\mathbf{x}_1 \in \mathbb{R}^d} \exp\left(i\left(\frac{m}{\epsilon}\mathbf{x}_1^2 - \epsilon V(\mathbf{x}_1)\right)\right) \exp\left(-i\frac{m}{\epsilon}(\mathbf{x}_b + \mathbf{x}_a) \cdot \mathbf{x}_1\right) d\mathbf{x}_1 \quad (50)$$

$$= \sqrt{2\pi}^{-d} \exp\left(i\left(\frac{m}{2\epsilon}(\mathbf{x}_b^2 + \mathbf{x}_a^2) - \epsilon V(\mathbf{x}_b)\right)\right) \hat{h}\left(\frac{m}{\epsilon}(\mathbf{x}_b + \mathbf{x}_a)\right) \quad (51)$$

and

$$h(\mathbf{x}_1) := \exp\left(i\left(\frac{m}{\epsilon}\mathbf{x}_1^2 - \epsilon V(\mathbf{x}_1)\right)\right). \quad (52)$$

Now

$$K_2(\mathbf{x}_b, \mathbf{x}_a; \epsilon) = \left(\frac{m}{2\pi i \epsilon} \sqrt{2\pi}\right)^d \exp\left(i\left(\frac{m}{2\epsilon}(\mathbf{x}_b^2 + \mathbf{x}_a^2) - \epsilon V(\mathbf{x}_b)\right)\right) \hat{h}\left(\frac{m}{\epsilon}(\mathbf{x}_b + \mathbf{x}_a)\right). \quad (53)$$

We call this kernel the *midpoint kernel*.

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

$$\hat{h}(\mathbf{k}) = \frac{i}{2k} \left(\hat{f}(k) - \hat{f}(-k)\right), \quad (54)$$

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 (54) is one-dimensional.

6 Quantum Harmonic Oscillator and Hydrogen-like Atom

The potential of the one-dimensional harmonic oscillator is

$$V(x) = \frac{m\omega_0^2}{2} x^2 \quad (55)$$

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

$$V(\mathbf{x}) = \frac{m\omega_0^2}{2}|\mathbf{x}|^2. \quad (56)$$

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

$$K(x_b, x_a; t) = \left(\frac{m\omega_0}{2\pi i \sin(\omega_0 t)} \right)^{1/2} \exp(iS_{\text{cl}}), \quad (57)$$

where S_{cl} is the classical action given by

$$S_{\text{cl}} = \frac{m\omega_0}{2 \sin(\omega_0 t)} ((x_b^2 + x_a^2) \cos(\omega_0 t) - 2x_b x_a). \quad (58)$$

By substituting the potential of the one-dimensional harmonic oscillator to equation (52) we obtain

$$h(x_1) = \exp\left(i \frac{m}{\epsilon} \left(1 - \frac{\epsilon^2 \omega_0^2}{2}\right) x_1^2\right). \quad (59)$$

Define

$$a := \frac{m}{\epsilon} \left(1 - \frac{\epsilon^2 \omega_0^2}{2}\right) \quad (60)$$

and assume that $a > 0$. Now

$$\hat{h}(k) = \frac{1}{2}(1+i) \frac{1}{\sqrt{a}} \exp\left(-i \frac{k^2}{4a}\right). \quad (61)$$

Similarly, in the three-dimensional case we have

$$\hat{h}(\mathbf{k}) = \frac{1}{4}(-1+i)a^{-3/2} \exp\left(-i \frac{k^2}{4a}\right) \quad (62)$$

using equation (54).

The potential of a hydrogen-like atom is

$$V(x) = -\frac{Z}{|x|} \quad (63)$$

in one dimension and

$$V(\mathbf{x}) = -\frac{Z}{|\mathbf{x}|} \quad (64)$$

in three dimensions. Here Z is the atomic number. The Trotter kernel for a hydrogen-like atom is computed by equation (10) and the midpoint kernel by equation (53).

7 Representation of the Path-Integral Kernel in Wavelet Bases

7.1 Interpolating Wavelets

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

$$\varphi(x) = \sum_{\alpha \in \mathbb{Z}} s[\alpha] \varphi(2^J x - \alpha) \quad (65)$$

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

$$\eta_{j_{\min}, k}(2^{-J-j_{\min}} p) = s_0[p - 2^J k] \quad (66)$$

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

$$\eta_{j_{\min}+1, k}(2^{-J-j_{\min}} p) = s_0[p - 2^{J-1} k] \quad (67)$$

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

$$\eta_{j_{\min}+1, k}(2^{-J-j_{\min}} p) = s_1[p - 2^{J-1} k] \quad (68)$$

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

$$\tilde{\eta}_{j_{\min}, \ell} = \tilde{\varphi}_{j_{\min}, \ell} = \delta(\cdot - 2^{-j_{\min}} \ell) \quad (69)$$

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

$$\tilde{\eta}_{j_{\min}+1, \ell} = \delta(\cdot - 2^{-j_{\min}-1} \ell) = \sum_{\beta \in \mathbb{Z}} \tilde{h}_{\beta} \delta(\cdot - 2^{-j_{\min}-1} (\beta + \ell)) \quad (70)$$

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

$$\tilde{\eta}_{j_{\min}+1, \ell} = \sum_{\beta \in \mathbb{Z}} \tilde{g}_{\beta} \delta(\cdot - 2^{-j_{\min}-1} (\beta + \ell - 1)) \quad (71)$$

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

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

$$K_{\mathbf{r}, \mathbf{q}} = \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \tilde{\zeta}_{\mathbf{r}}(\mathbf{y}) K(\mathbf{y}, \mathbf{x}; \epsilon) \zeta_{\mathbf{q}}(\mathbf{x}) d\mathbf{x} d\mathbf{y}. \quad (72)$$

It follows from equation (12) 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

$$K_{\mathbf{r}, \mathbf{q}} = \int_{\mathbb{R}^d} K(2^{-j_{\min}} \ell, \mathbf{x}; \epsilon) \zeta_{\mathbf{q}}(\mathbf{x}) d\mathbf{x}. \quad (73)$$

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

$$\int_{\mathbb{R}} K(y, x; \epsilon) \zeta_q(x) dx \approx 2^{-j_{\min}-J} \sum_{p \in \mathbb{Z}} K(y, 2^{-j_{\min}-J} p; \epsilon) s_{t(q)}(p - 2^{J-t(q)} k) \quad (74)$$

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

$$t(q) := \begin{cases} 1 & \text{if } q \in G_{j_{\min}+1} \\ 0 & \text{if } q \in G_{j_{\min}}. \end{cases} \quad (75)$$

For the three-dimensional case define

$$T(\mathbf{q}) := \begin{cases} 1 & \text{if } \mathbf{q} \in G_{j_{\min}+1} \\ 0 & \text{if } \mathbf{q} \in G_{j_{\min}} \end{cases} \quad (76)$$

and

$$t_i(\mathbf{q}) := \begin{cases} 1 & \text{if } \mathbf{q} \in G_{j_{\min}+1} \text{ and } 2^{j_{\min}+1} \mathbf{q}[i] \text{ odd} \\ 0 & \text{otherwise} \end{cases} \quad (77)$$

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

$$s_{\mathbf{t}}[\mathbf{z}] := s_{t[1]}[\mathbf{z}[1]] s_{t[2]}[\mathbf{z}[2]] s_{t[3]}[\mathbf{z}[3]]. \quad (78)$$

Now we can approximate

$$\int_{\mathbb{R}^3} K(\mathbf{y}, \mathbf{x}; \epsilon) \zeta_{\mathbf{q}}(\mathbf{x}) d\mathbf{x} \approx 2^{-3(j_{\min}+J)} \sum_{\mathbf{p} \in \mathbb{Z}^3} K(\mathbf{y}, 2^{-j_{\min}-J} \mathbf{p}; \epsilon) s_{\mathbf{t}(\mathbf{q})}[\mathbf{p} - 2^{J-T(\mathbf{q})} \mathbf{k}] \quad (79)$$

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 (65) 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

$$\varphi(x) = 2^{J/2} \sum_{\alpha \in \mathbb{Z}} w[\alpha] \varphi(2^J x - \alpha) \quad (80)$$

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

$$K_{j,k,j',k'} = \int_{\mathbb{R}} \int_{\mathbb{R}} \zeta_{j,k}(y) K(y, x; \epsilon) \zeta_{j',k'}(x) dx dy \quad (81)$$

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

8 Application to the Harmonic Oscillator and Hydrogen Atom

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.

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 $(1/4)\{-48, \dots, 48\}$ for one-level calculations and $(1/4)\{-48, \dots, 48\} \cup (1/8)\{-5, \dots, 5\}$ 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.

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 we use the basis $\{(2, -48), \dots, (2, 48)\}$ and for the two-level calculations $\{(1, -24), \dots, (1, 24)\} \cup \{(2, -6), \dots, (2, 6)\}$. We set the mother scaling function resolution to $J = 5$. The resulting ground state energies 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 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. 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 method described in section 4 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 $\{-10, \dots, 10\}^3$ 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. 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 $(1/2)\{-9, \dots, 9\} \cup (1/4)\{-4, \dots, 4\}$. The function $\hat{h}(\mathbf{k})$ for the midpoint kernel is calculated with formula (54). We have to invert the sign of the midpoint kernel (53) 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

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	-	-

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.

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.

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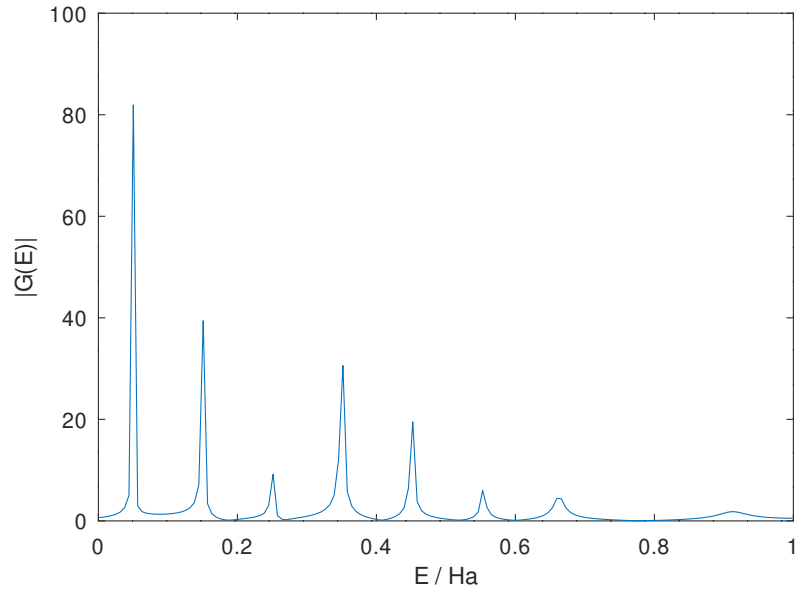


Figure 1: Energy spectrum of the one-dimensional harmonic oscillator computed with the exact kernel.

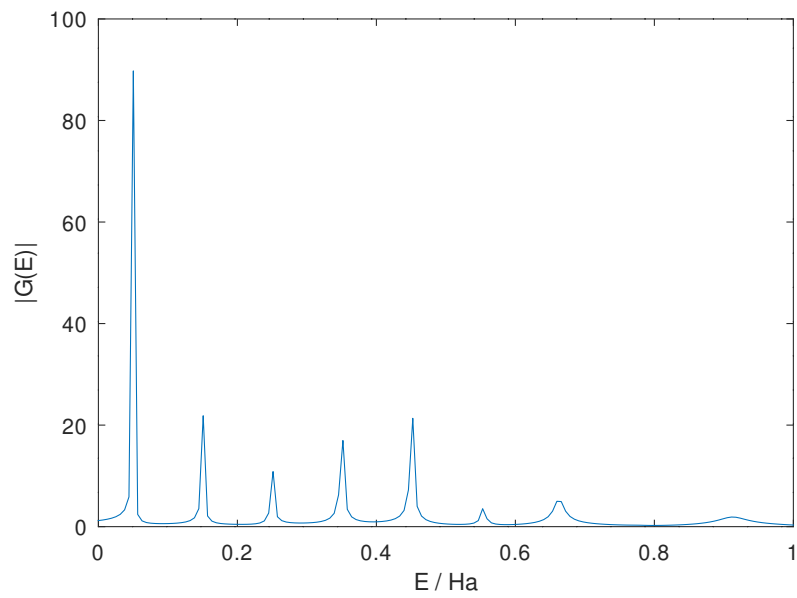


Figure 2: Energy spectrum of the one-dimensional harmonic oscillator computed with the midpoint kernel.

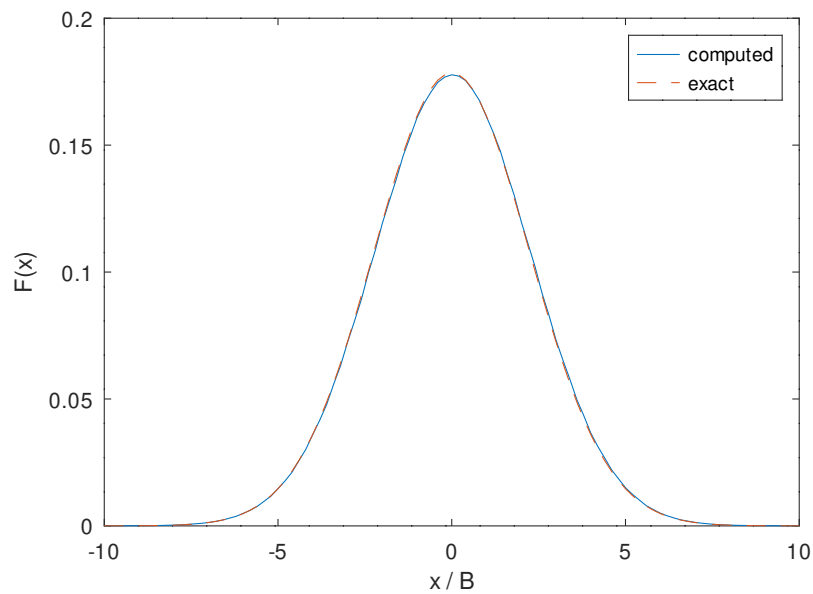


Figure 3: Probability density function $F(x) = |\psi(x)|^2$ of the one-dimensional harmonic oscillator computed with the exact kernel.

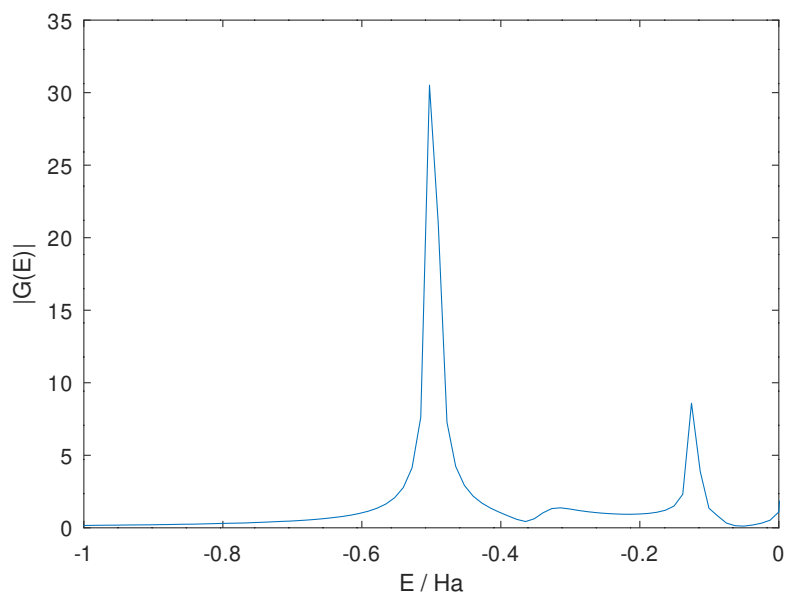


Figure 4: Energy spectrum of the hydrogen atom computed with the Trotter kernel in one dimension.

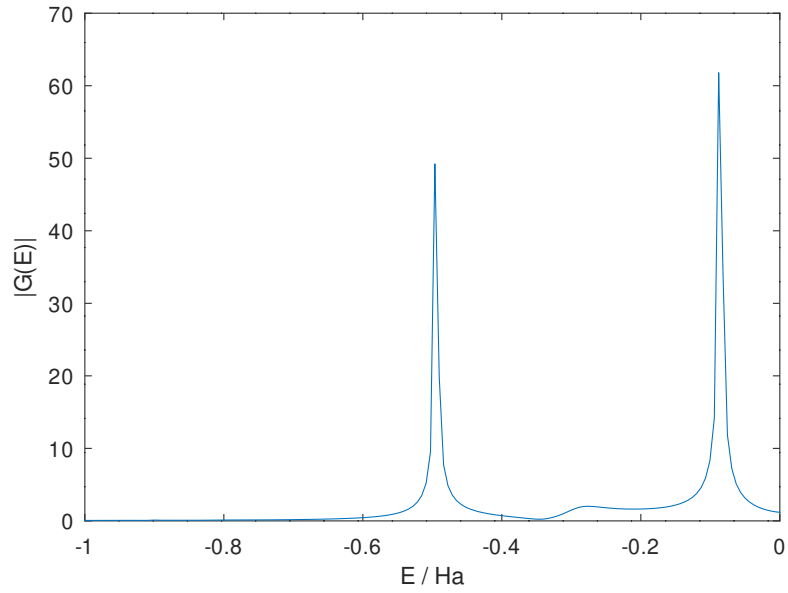


Figure 5: Energy spectrum of the hydrogen atom computed with the midpoint kernel in one dimension.

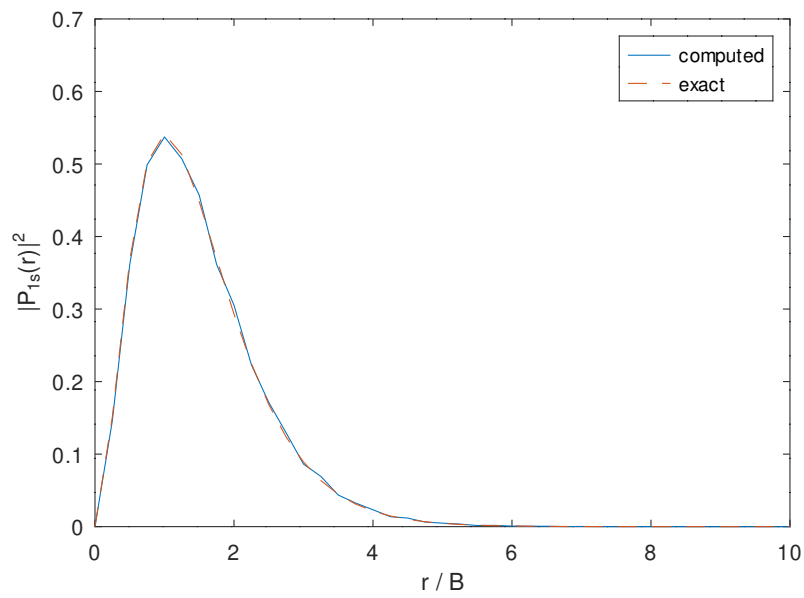


Figure 6: Radial probability density function $|P_{1s}(r)|^2$ of the hydrogen atom computed with the midpoint kernel in one dimension.

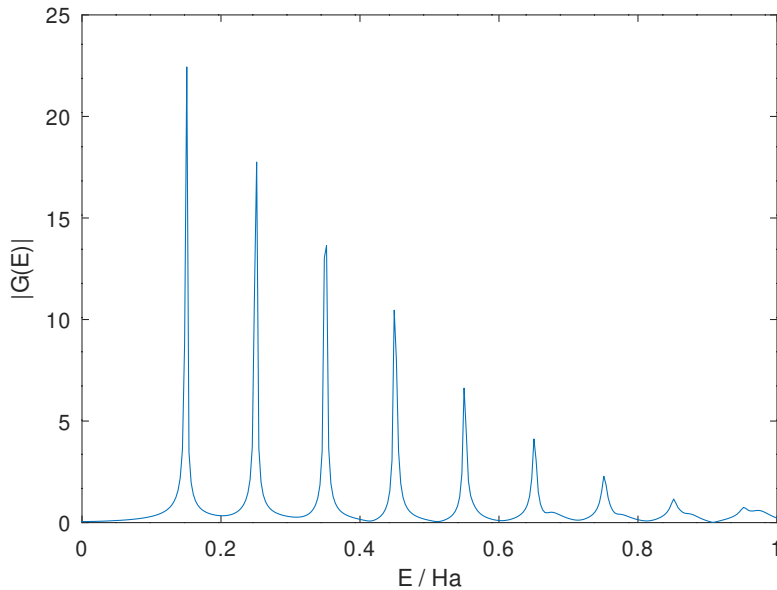


Figure 7: Energy spectrum of the three-dimensional harmonic oscillator calculated with the midpoint kernel.

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