Time-Dependent Schrödinger Equation with Magnetic Field

Etienne Corminboeuf

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Contents

1 Introduction

In this report we consider a spinless particle in $\mathbb{R}^d$ with mass $m \in \mathbb{R}_{\geq 0}$ and charge $e \in \mathbb{R}$ in a homogeneous magnetic field $B(t)$. We follow the notation introduced in the paper by Gradinaru and Rietmann and quickly recap the important elements. For a full derivation please consult [1].

1.1 Mathematic model

In quantum mechanics, the time evolution of a particle subject to a magnetic field is governed by the Pauli equation

$$i\hbar\partial_t \Psi(x,t) = H_P(t)\Psi(x,t) \tag{1}$$

$$H_P(t) := \frac{1}{2m}\sum_{k=1}^{d}(p_k - eA_k(x,t))^2 + e\phi(x,t) + \tilde{V}(x,t) \tag{2}$$

where $\tilde{V}(x,t)$ is some external potential. The magnetic field 2-form dA associated with $B(t)$ is independent of x because of the homogeneity of $B(t)$ and we can thus rewrite the magnetic vector potential

to

$$A(x,t) := \frac{1}{2} B_{jk}(t) x^j \mathrm{d}x^k, \tag{3}$$

where $B(t) = (B_{jk}(t))_{j,k=1}^d$ is a real, skew-symmetric matrix. Using the operators

$$L_{jk} := x_j p_k - x_k p_j \tag{4}$$

$$H_B(t) := -\sum_{j,k=1}^{d} B_{jk}(t) L_{jk} \tag{5}$$

the Pauli-Hamiltonian takes the form

$$H_P(t) = \frac{1}{2m}\left(\hbar^2(-\Delta) - e\sum_{1\leqslant j<k\leqslant d} B_{jk}(t)L_{jk} + \frac{e^2}{4}\|B(t)x\|^2_{\mathbb{R}^d}\right) + e\phi(x,t) + \tilde{V}(x,t). \tag{6}$$

1.2 Numerical model

We introduce $\epsilon^2 := \hbar$ and redefine t, x and B to find the simplified form

$$H_P(t) = -\Delta + H_B(t) + V(x,t) \tag{7}$$

where $V(x,t) := \frac{1}{2m}\frac{e^2}{4}\|B(t)x\|^2_{\mathbb{R}^d} + e\phi(x,t) + \tilde{V}(x,t)$ can be considered to be a total effective potential. The Schrödinger equation

$$i\epsilon^2 \partial_t \Psi(x,t) = H_P(t)\Psi(x,t) \tag{H}$$

is then split up into three separate parts that can be solved numerically.

$$i\epsilon^2 \partial_t \Psi = -\Delta\Psi \tag{K}$$

$$i\epsilon^2 \partial_t \Psi = H_B(t)\Psi \tag{M}$$

$$i\epsilon^2 \partial_t \Psi = V(x,t)\Psi \tag{P}$$

(K) can be solved discretely in Fourier-space and (P) by pointwise multiplication with $e^{-i/\epsilon^2 \int_{t_0}^t dt V(x,t)}$. (M) is reduced to the linear differential equation

$$\frac{d}{dt} y(t) = B(t) y(t) \tag{B}$$

[2] proves the existence of a flow map $U(t,t_0)$ which is a solution to (B). The unitary representation

$$\rho : SO(d) \longrightarrow U(L^2(\mathbb{R}^d)) \tag{8}$$

$$R \longmapsto (\rho(R)\Psi)(x) = \Psi(R^{-1}x) \tag{9}$$

maps the solution $U(t,t_0)$ of (B) to a solution of (M). The proof of this statement can be found in [1]. The exact flow map $U(t,t_0)$ is approximated through a Magnus expansion proposed by Blanes and Moan [3]. Direct calculation shows $[-\Delta,\, H_B(t)] = 0$. Thus the flow maps solving (K) and (M) yield a solution to the differential equation

$$i\epsilon^2 \partial_t \Psi = (-\Delta + H_B(t))\Psi \tag{K+M}$$

in the following way: Denote the solutions to (K) and (M) by $\Phi_{-\Delta}$ and Φ_{H_B} respectively. This means that the flow map to (K) satisfies

$$i\frac{d}{dt}\Phi_{-\Delta}(t,t_0) = -\Delta\Phi_{-\Delta}(t,t_0), \quad \Phi_{-\Delta}(t_0,t_0) = id, \tag{10}$$

and analogously for the flow map to (M). The flow map $\Phi_{-\Delta+H_B}$ which is a solution to (K+M) then follows as a simple multiplication

$$\Phi_{-\Delta+H_B}(t,t_0) = \Phi_{H_B}(t,t_0)\Phi_{-\Delta}(t,t_0) = \Phi_{-\Delta}(t,t_0)\Phi_{H_B}(t,t_0). \tag{11}$$

Finally, combining the solutions to (K+M) and (P) using a splitting scheme leads to a solution of H.

1.3 Splitting

Consider a splitting scheme with the coefficients (a_i, b_i) for $1 \leq i \leq n$ and the time grids

$$t_i = t_0 + (t-t_0)\sum_{j=1}^{i} b_j \quad \text{and} \quad s_i = t_0 + (t-t_0)\sum_{j=1}^{i} a_j \tag{12}$$

to an initial time t_0. [1] derives an explicit expression of the solution to H as follows:

$$\Phi_H\left(t_0+Nh,t_0\right) \approx \left(\prod_{j=0}^{N-1}\prod_{i=0}^{n-1} \Phi_{-\Delta}\left(t_{i+1},t_i\right)\Phi_{\rho(U(t_0+Nh,t_i+jh))V}\left(s_{i+1}+jh,s_i+jh\right)\right)\Phi_{H_B}\left(t_0+Nh,t_0\right) \tag{13}$$

where h is the splitting time step, ρ the representation defined in eq. 8 and $U(t,t_0)$ the exact flow map to (B).
To simplify the numerical calculations the propagator for the potential part $\Phi_V = \exp(-i\int_{t_0}^{t} V(x,s)ds)$ can be rewritten using the definition $V(x,t) = \|B(t)x\|^2_{\mathbb{R}^d} + \phi(x,t)$ to

$$\int_{t_0}^{t} V(x,s)ds = \langle x, \left(-\int_{t_0}^{t} B^2(s)ds\right)x\rangle + \int_{t_0}^{t}\phi(x,s)ds. \tag{14}$$

2 Implementation

The method summarised above was implemented into the WaveBlocksND project, developed by Bourquin and Gradinaru [4]. To that avail we created a new *FourierMagneticPropagator*-class, based on the existing *FourierPropagator*-class. The full class code can be found in Appendix A. In this section, we present the *'postpropagate'*-function which carries the implementation of section 1 and explain its approach.
The *FourierMagneticPropagator*-class carries the header portrayed in figure 1. The code of the *postpropagate*-function is summarised in Algorithm 1 and can also be found in Appendix A. It implements the propagator from equation 1 and is based on Algorithm 1 from [1]. Its header reads as portrayed in figure 2.

The flow map ρ from equation 8 effectively acts as a rotation. These rotations could not directly be applied onto the potential V or the wavefunction Ψ but had to be realised via a rotation of the

class WaveBlocksND.**FourierMagneticPropagator**(*parameters*, *potential*, *initial_values*)

This class can numerically propagate given initial values $\Psi(x_0, t_0)$ on a potential hyper[source] surface $V(x)$, in presence of a magnetic field. The propagation is done with a splitting of the time propagation operator $\exp(-\frac{i}{\varepsilon^2}\tau H)$. Available splitting schemes are implemented in SplittingParameters.

Figure 1: Documentation-Header of the FourierMagneticPropagator Class.

post_propagate(*tspan*) [source]

Given an initial wavepacket Ψ_0 at time $t = 0$, calculate the propagated wavepacket Ψ at time $tspan[0]$. We perform $n = \lceil tspan[0]/dt \rceil$ steps of size dt.

Parameters: **tspan** – ndarray consisting of end time at position 0, other positions are irrelevant.

Figure 2: Header of the postpropagate-function.

underlying grid X. More precisely, the operation $(\rho(R)A)(x) = A(R^{-1}x)$ requires us to first rotate the grid X by R^{-1} and then evaluate the quantity A on the rotated grid. Because X is a class member in WaveBlocksND, after the evaluation of A on $R^{-1} \cdot X$ we need to reverse the above rotation to return to the original state.
Because of the rotational invariance of the first term in equation 14, in the term $\Phi_{\rho(U(t_0+Nh,t_i+jh))V}$ only the electric potential ϕ needs to be subjected to such a rotation.

3 Results

//include convergence plots here
//also include wavefct plot and discuss similarities to paper

4 Summary and Conclusion

Appendices

A Code

```
r"""The WaveBlocks Project

This file contains the Fourier Magnetic Propagator class. The wavefunction
:math:`\Psi` is propagated in time with a splitting of the
exponential :math:`\exp(-\frac{i}{\varepsilon^2} \tau H)`.

```

```
@author: R. Bourquin
@copyright: Copyright (C) 2012, 2016 R. Bourquin
@license: Modified BSD License
"""

from numpy import array, complexfloating, dot, exp, eye, zeros, shape
from numpy.fft import fftn, ifftn
from scipy.linalg import expm

from WaveBlocksND.BlockFactory import BlockFactory
from WaveBlocksND.Propagator import Propagator
from WaveBlocksND.KineticOperator import KineticOperator
from WaveBlocksND.MagneticField import MagneticField
from WaveBlocksND.SplittingParameters import SplittingParameters

__all__ = ["FourierMagneticPropagator"]


class FourierMagneticPropagator(Propagator, SplittingParameters):
    r"""This class can numerically propagate given initial values :math:`\Psi(x_0, t_0)` on
    a potential hyper surface :math:`V(x)`, in presence of a magnetic field. The propagation is done with a splitting
    of the time propagation operator :math:`\exp(-\frac{i}{\varepsilon^2} \tau H)`.
    Available splitting schemes are implemented in :py:class:`SplittingParameters`.
    """

    def __init__(self, parameters, potential, initial_values):
        r"""Initialize a new :py:class:`FourierMagneticPropagator` instance. Precalculate the
        the kinetic operator :math:`T_e` and the potential operator :math:`V_e`
        used for time propagation.

        :param parameters: The set of simulation parameters. It must contain at least
                           the semi-classical parameter :math:`\varepsilon` and the
                           time step size :math:`\tau`.
        :param potential: The potential :math:`V(x)` governing the time evolution.
        :type potential: A :py:class:`MatrixPotential` instance.
        :param initial_values: The initial values :math:`\Psi(\Gamma, t_0)` given
                               in the canonical basis.
        :type initial_values: A :py:class:`WaveFunction` instance.

        :raise: :py:class:`ValueError` If the number of components of :math:`\Psi` does not match the
                           number of energy surfaces :math:`\lambda_i(x)` of the potential.

        :raise: :py:class:`ValueError` If the number of components of :math:`\Psi` does not match the dimension of the magnetic field :math:`\vec{B}(x)`.

        :raise: :py:class:`ValueError` If the dimensions of the splitting scheme parameters :math:`a` and :math:`b` are not equal.
        """
        # The embedded 'MatrixPotential' instance representing the potential 'V'.
        self._potential = potential

        # The initial values of the components '\psi_i' sampled at the given grid.
        self._psi = initial_values
```

```
58
59          if self._potential.get_number_components() != self._psi.get_number_components
    ():
60              raise ValueError("Potential dimension and number of components do not
    match.")
61
62          # The time step size.
63          self._dt = parameters["dt"]
64
65          # Final time.
66          self._T = parameters["T"]
67
68          # The model parameter '\varepsilon'.
69          self._eps = parameters["eps"]
70
71          # Spacial dimension d
72          self._dimension = parameters["dimension"]
73
74          # The position space grid nodes '\Gamma'.
75          self._grid = initial_values.get_grid()
76
77          # The kinetic operator 'T' defined in momentum space.
78          self._KO = KineticOperator(self._grid, self._eps)
79
80          # Exponential '\exp(-i/2*eps^2*dt*T)' used in the Strang splitting.
81          # not used
82          self._KO.calculate_exponential(-0.5j * self._dt * self._eps**2)
83          self._TE = self._KO.evaluate_exponential_at()
84
85          # Exponential '\exp(-i/eps^2*dt*V)' used in the Strang splitting.
86          # not used
87          self._potential.calculate_exponential(-0.5j * self._dt / self._eps**2)
88          VE = self._potential.evaluate_exponential_at(self._grid)
89          self._VE = tuple([ve.reshape(self._grid.get_number_nodes()) for ve in VE])
90
91          # The magnetic field
92          self._B = MagneticField(parameters["B"])
93          # check if magnetic field and potential are of same dimension
94          if self._B.get_dimension() != self._dimension:
95              raise ValueError("Spacial dimension of potential and magnetic field must
    be the same")
96
97          #precalculate the splitting needed
98          self._a, self._b = self.build(parameters["splitting_method"])
99          if shape(self._a) != shape(self._b):
100             raise ValueError("Splitting scheme shapes must be the same")
101
102         # Get inital data as function
103         packet_descr = parameters["initvals"][0]
104         self._initalpacket = BlockFactory().create_wavepacket(packet_descr)
105
106
107     # TODO: Consider removing this, duplicate
108     def get_number_components(self):
109         r"""Get the number :math:`N` of components of :math:`\Psi`.
110
111         :return: The number :math:`N`.
112         """
```

```
        return self._potential.get_number_components()


    def get_wavefunction(self):
        r"""Get the wavefunction that stores the current data :math:`\Psi(\Gamma)`.

        :return: The :py:class:`WaveFunction` instance.
        """
        return self._psi


    def get_operators(self):
        r"""Get the kinetic and potential operators :math:`T(\Omega)` and :math:`V(\Gamma)`.

        :return: A tuple :math:`(T, V)` containing two ``ndarrays``.
        """
        # TODO: What kind of object exactly do we want to return?
        self._KO.calculate_operator()
        T = self._KO.evaluate_at()
        V = self._potential.evaluate_at(self._grid)
        V = tuple([v.reshape(self._grid.get_number_nodes()) for v in V])
        return (T, V)


    @staticmethod
    def _Magnus_CF4(tspan, B, N, *args):
        r"""Returns the  Fourth Order Magnus integrator :math:`\Omega(A)` according to [#]_.

        :param tspan: Full timespan of expansion.

        :param B: Magnetic field matrix :math:`B(t) = (B_{j,k}(t))_{1 \leq j, k \leq d}`.

        :param N: Number of timesteps for the expansion.

        :param *args: Additional arguments for the magnetic field :math:`B(t, *args)`

        .. [#] S. Blanes and P.C. Moan. "Fourth- and sixth-order commutator-free Magnus integrators for linear and non-linear dynamical systems". Applied Numerical Mathematics, 56(12):1519 - 1537, 2006.
        """
        # Magnus constants
        c1 = 0.5*(1.0 - 0.5773502691896258)
        c2 = 0.5*(1.0 + 0.5773502691896258)
        a1 = 0.5*(0.5 - 0.5773502691896258)
        a2 = 0.5*(0.5 + 0.5773502691896258)

        R = 1.*eye( len( B(1.*tspan[0], *args) ) )
        h = (tspan[1]-tspan[0]) / (1.*N)
        for k in range(N):
            t0 = k*h + tspan[0]
            t1 = t0 + c1*h
            t2 = t0 + c2*h
            B1 = B(t1, *args)
            B2 = B(t2, *args)
            R = dot(expm(a1*h*B1+a2*h*B2), dot(expm(a2*h*B1+a1*h*B2), R))
```

```
166
167         return R
168
169
170     def post_propagate(self, tspan):
171         r"""Given an initial wavepacket :math:`\Psi_0` at time :math:`t=0`, calculate
    the propagated wavepacket :math:`\Psi` at time :math:`tspan \[ 0 \]`. We perform :
    math:`n = \lceil tspan\[ 0 \] /dt \rceil` steps of size :math:`dt`.
172
173         :param tspan: :py class:`ndarray` consisting of end time at position 0, other
    positions are irrelevant.
174         """
175
176         # (ignoriere tspan[0])
177         nsteps = int(tspan[0] / self._dt + 0.5)
178         print("Perform " + str(nsteps) + " steps from t = 0.0 to t = " + str(tspan[0])
    )
179
180
181         # Magnetfeld Matrix B(t)
182         B = lambda t: self._B(t)
183
184         #how many components does Psi have
185         N = self._psi.get_number_components()
186
187         #start time t_0 = 0?
188         t0 = 0
189         t_a = t0
190         t_b = t0
191
192         #calculate R = U(t0 + N*h, t0)
193         #Use N = n_steps to account for large time difference
194         t_interval = array([t0, tspan[0]])
195         R = FourierMagneticPropagator._Magnus_CF4(t_interval, B, nsteps)
196
197         # rotate the grid by the transpose of R
198         self._grid.rotate(R.T)
199
200         # Compute rotated initial data
201         X = self._grid.get_nodes(flat=True)
202         values = self._initalpacket.evaluate_at(X, prefactor=True)
203         values = tuple([val.reshape(self._grid.get_number_nodes()) for val in values])
204         self._psi.set_values(values)
205
206         self._grid.rotate(R)
207
208         #calculate the necessary timesteps
209         for j in range(nsteps):
210             for i in range(len(self._a)):
211                 # Integral -\int_{tspan[0]}^{tspan[1]}B^2(s)ds und zugehÃ¶rige
    Propagation
212                 # (siehe Paper, Remark 3.1)
213                 minus_B_squared = lambda t: (-1.0) * dot(B(t), B(t))
214                 A = 1.0 / 8.0 * MagneticField.matrix_quad(minus_B_squared, t_a, t_a +
    self._a[i]*self._dt)
215
216                 X = self._grid.get_nodes(flat=True)
217                 VB = sum(X * dot(A, X))
```

```
                VB = VB.reshape(self._grid.get_number_nodes())
                prop = exp(-1.0j / self._eps**2 * VB) # ev. -0.5j durch -1j ersetzen
    ...

                values = self._psi.get_values()
                values = [prop * component for component in values]

                self._potential.calculate_exponential(-1.0j *  self._a[i]*self._dt /
    self._eps**2)

                self._grid.rotate(R.T)
                VE = self._potential.evaluate_exponential_at(self._grid)
                self._VE = tuple([ve.reshape(self._grid.get_number_nodes()) for ve in
    VE])

                #apply it
                values = [self._VE * component for component in values]
                self._grid.rotate(R)

                t_interval[0] = t_b
                t_interval[1] = t_b + self._b[i]*self._dt

                U = (FourierMagneticPropagator._Magnus_CF4(t_interval, B, 1)).T
                R = dot(R , U)
                if(R.shape != U.shape):
                    raise ValueError("Shapes of R and U do not match")

                #check for obsolete splitting steps
                if(self._b[i] != 0):
                    values = [fftn(component) for component in values]

                    # Apply the kinetic operator
                    self._KO = KineticOperator(self._grid, self._eps)
                    self._KO.calculate_exponential(-0.5j * self._eps**2 * self._b[i]*
    self._dt)

                    TE = self._KO.evaluate_exponential_at()
                    values = [TE * component for component in values]

                    # Go back to real space
                    values = [ifftn(component) for component in values]

                #Apply
                self._psi.set_values(values)

                #update t_a and t_b
                t_a = t_a + self._a[i]*self._dt
                t_b = t_b + self._b[i]*self._dt

        return tspan[0]


    def propagate(self, tspan):
        r"""This method does nothing.
        """
```

References

[1] V. Gradinaru and O. Rietmann. *A High-Order Integrator for the Schrödinger Equation with Time-Dependent, Homogeneous Magnetic Field*. Unpublished article, ETH Zürich, submitted for publication, 2020.

[2] B. Simon and M. Reed. *Fourier Analysis, Self-Adjointness, Volume 2* of *Methods of Modern Mathematical Physics*. Academic Press, Boston, 1975.

[3] S. Blanes and P.C. Moan. *Fourth- and sixth-order commutator-free Magnus integrators for linear and non-linear dynamical systems*. Applied Numerical Mathematics, 56(12):1519 - 1537, 2006.

[4] R. Bourquin and V. Gradinaru. *WaveBlocks: Reusable building blocks for simulations with semiclassical wavepackets*, GitHub, URL: `https://github.com/WaveBlocks/WaveBlocksND`, 2010 - 2016.

Algorithm 1: PostPropagate Function

Data: *As arguments to the function:* class instance $self$; end time t.
As arguments to the class instance: step width dt; meshgrid X; initial wave function Ψ_0; potential V; magnetic field B; number of components of the wavefunction N; quantisation parameter ϵ; splitting method with coefficients $(a_i, b_i)_{i=1}^{n}$; end time of simulation T; dimension d; frequency of writing to disk w_n.

Result: Computes wavepacket at time t and saves it to class member. **Returns:** End time t.

define stepwidth: $n_{steps} = \lceil t/dt \rceil$;
define time grids: $t_a = t_0$, $t_b = t_0$;
calculate flow map $R = U(t_0 + N \cdot dt, t_0)$;
rotate the grid by R^T ;
evaluate initial data on rotated grid and save to wavefunction Ψ;
rotate grid back ;
for *j = 0 to nsteps* **do**
    for *i = 0 to dim(a)* **do**
        potential propagator $\Phi_V = \Phi_B \cdot \Phi_\phi$:
            calculate magnetic field propagator $\Phi_B = \exp(-i\langle x, (\int_{t_a}^{t_a + a_i \cdot dt} B^2(s)ds)x\rangle)$;
            apply propagator to Ψ ;
            rotate grid by R^T ;
            calculate electric and external potential propagator $\Phi_\phi = \exp(-i \int_{t_a}^{t_a + a_i \cdot dt} (\phi(x, s) + V_{ext})ds)$;
            apply propagator to Ψ on rotated grid ;
            rotate grid back ;
        calculate flow map $R = R \cdot U^{-1}(t_b + b_i \cdot dt, t_b)$;
        kinetic propagator $\Phi_{-\Delta}$:
            Fast-Fourier-Transform Ψ to Fourier space ;
            calculate the kinetic propagator $Phi_{-\Delta}$;
            apply propagator to $\mathcal{FFT}(\Psi)$;
            Inverse-FFT Ψ to real space ;
        update time grids: $t_a = t_a + a_i \cdot dt$, $t_b = t_b + b_i \cdot dt$;
    end
end
return t