

FourierMagneticPropagator — WaveBlocksND

devel documentation

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FourierMagneticPropagator¶

About the FourierMagneticPropagator class¶

The WaveBlocks Project

@author: R. Bourquin @copyright: Copyright (C) 2010, 2011, 2012, 2013, 2014, 2015, 2016 R. Bourquin @license: Modified BSD License

Inheritance diagram¶

```
digraph inheritance0585146a3b { rankdir=LR; size="8.0, 12.0"; "Wave-  
BlocksND.FourierMagneticPropagator.FourierMagneticPropagator" [font-  
name="Vera Sans, DejaVu Sans, Liberation Sans, Arial, Helvetica,  
sans",fontsize=10,height=0.25,shape=box,style="setlinewidth(0.5)",tooltip="This  
class can numerically propagate given initial values :math:'\Psi(x_0,  
t_0)' on"]; "WaveBlocksND.Propagator.Propagator" -> "WaveBlock-  
sND.FourierMagneticPropagator.FourierMagneticPropagator" [arrow-  
size=0.5,style="setlinewidth(0.5)"]; "WaveBlocksND.SplittingParameters.SplittingParameters"  
-> "WaveBlocksND.FourierMagneticPropagator.FourierMagneticPropagator" [ar-  
rowsize=0.5,style="setlinewidth(0.5)"]; "WaveBlocksND.Propagator.Propagator"  
[fontname="Vera Sans, DejaVu Sans, Liberation Sans, Arial, Helvetica,  
sans",fontsize=10,height=0.25,shape=box,style="setlinewidth(0.5)",tooltip="Propagators  
can numerically simulate the time evolution of quantum states"]; "WaveBlock-  
sND.SplittingParameters.SplittingParameters" [fontname="Vera Sans, DejaVu  
Sans, Liberation Sans, Arial, Helvetica, sans",fontsize=10,height=0.25,shape=box,style="setlinewidth(0.5)"];  
}
```

Class documentation¶

`class WaveBlocksND.FourierMagneticPropagator(parameters, potential, initial_values)[source]`¶

../_images/math/09ed461798fa50f983c7f98

This class can numerically propagate given initial values

../_images/math/947b2e7cf74785c545d567645fb43e1310e3b227.png

on a potential hyper surface, in presence of a magnetic field. The propagation is done with a splitting of the time propagation

../_images/math/06bd4236d9ab66809a1626d5c16887acd3db060e.png

operator. Available splitting schemes are implemented in `SplittingParameters`.

`__init__(parameters, potential, initial_values)[source]`¶

Initialize a new `FourierMagneticPropagator` instance. Pre-

../_images/math/f5339fd8776a3b7a951bfacc10f6c264c2722c

calculate the the kinetic operator and the potential

../_images/math/dd50200d238d34d8a9c9a131b57883840d9a6980.png

operator used for time propagation.

Parameters:

- **parameters** – The set of simulation parameters. It must contain at least the semi-classical parameter

../_images/math/3cb373a8030ad846aed7b1ee45bab27b1377

and the time

../_images/math/557d5fad862c9046d26e1a930f45a

step size

- **potential** (A `MatrixPotential` instance.) –

../_images/math/947b2e7cf74785c545d56764

The potential governing the time evolution.

- **initial_values** (A `WaveFunction` instance.) – The

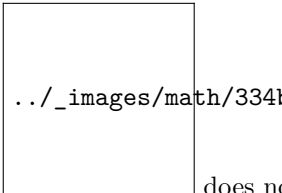
../_images/math/64b7a5c038df3580d26fd4dd7

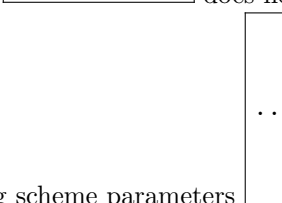
initial values given in the canonical basis.

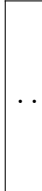
../_images/math/3341

Raise:

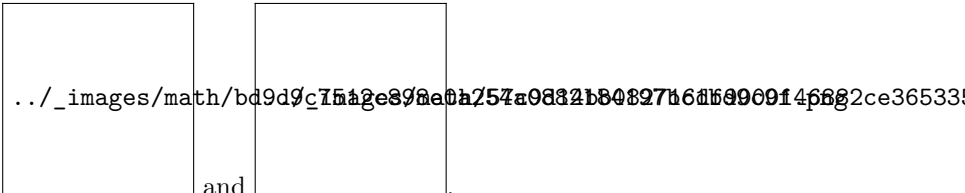
ValueError If the number of components of does not



Raise: ValueError If the number of components of  does not

Raise: ValueError If the dimensions of the splitting scheme parameters 

Parameters: **method** – A string specifying the method for time integration.



Returns: Two arrays  and .

Method	Order	Authors	Reference
LT	1	Lie/Trotter	[1], [3] page 42, c
S2	2	Strang	[2], [3] page 42, c
SS	2	Strang	[2], [3] page 42, c
PRKS6	4	Blanes/Moan	[4] page 318, tab
BM42	4	Blanes/Moan	[4] page 318, tab
Y4	4	Yoshida	[5], [3] page 40, c
Y61	6	Yoshida	[5], [3] page 144,
BM63	6	Blanes/Moan	[4] page 318, tab
KL6	6	Kahan/Li	[6], [3] page 144,
KL8	8	Kahan/Li	[6], [3] page 145,
KL10	10	Kahan/Li	[6], [3] page 146,

[1] H.F. Trotter, “On the product of semi-groups of operators”, Proc. Am. Math. Soc.10 (1959) 545-551.

[2] (1, 2) G. Strang, “On the construction and comparison of difference schemes”, SIAM J. Numer. Anal. 5

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- [3] (1, 2, 3, 4, 5, 6, 7, 8) E. Hairer, C. Lubich, and G. Wanner, “Geometric Numerical Integration - Structu
-
- [4] (1, 2, 3) S. Blanes and P.C. Moan, “Practical Symplectic Partitioned Runge-Kutta and Runge-Kutta-Ny
-
- [5] (1, 2) H. Yoshida, “Construction of higher order symplectic integrators”, Phys. Lett. A 150 (1990) 262-2
-
- [6] (1, 2, 3) W. Kahan and R.-c. Li, “Composition constants for raising the orders of unconventional schem
-

build(*method*)¶

../_images/math/f4170ed8938b79490d89238

get_number_components()[*source*]¶ Get the number

../_images/math/334b0728f25dd84a28e483181038a307ea6e483e.png

of components of

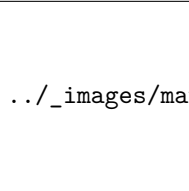
../_images/math/f4170ed8938b79490d8923857962695514a8e4c

Returns: The number

get_operators()[*source*]¶ Get the kinetic and potential operators

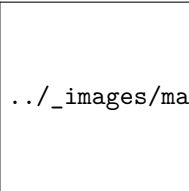
../_images/math/ac3f00803e12a5e103498251675e28e05402e076268c8c7871b99f3c2.png

and



../_images/math/93dc9ee713f6b766cbb69993fe73da97734012f8.png

Returns: A tuple containing two `ndarrays`.

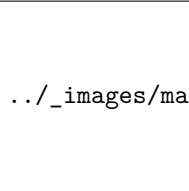


../_images/math/947b2e7cf74785c545d567645fb43e1310

`get_potential()`¶ Returns the potential used for time propagation.

Returns: A `MatrixPotential` subclass instance.

`get_wavefunction()[source]`¶ Get the wavefunction that stores the cur-



../_images/math/7e3449b74b914c8f5312bb21cc4c91a78e529e3f.png

rent data

Returns: The `WaveFunction` instance.

`intsplitt(psi1, psi2, a, b, tspan, N, args1=[], args2=[])`¶
Compute a single, full propagation step by operator splitting.

Parameters:

- **psi1** – First evolution operator

../_images/math/f59ab6519c20d5ec43c63697e7603d2c1a6f

- **psi2** – Second evolution

../_images/math/e1a342b133bb7797223252052133

operator

- **a** – Parameters for evolution

../_images/math/f59ab6519c20d5ec43c63697e7603d2c

with

- **b** – Parameters for evolution

../_images/math/e1a342b133bb7797223252052133e810

with

- **tspan** – Timespan

../_images/math/5ec053cf70dc1c98cc297322250569eda193

of a single, full

splitting step

- **N** – Number of substeps to perform
- **args1** – Additional optional

../_images/math/f59ab6519c20d5ec43c63697e

arguments of

- **args2** – Additional optional

../_images/math/e1a342b133bb7797223252052

arguments of

Note

The values for `args1` and `args2` have to be of type `list` even in case of single items.

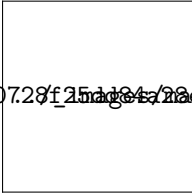
Parameters:	method – A string specifying the method for time integration.
Returns:	The order of this method.

`order(method)`¶

`post_propagate(tspan)[source]`¶ Given an initial wavepacket

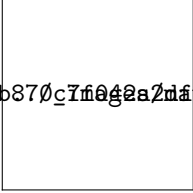


at time , calculate the propagated



../_images/math/334b0728f25d184/284493870a3a3a3b0d7e237b6c1da1dd20c914a.png

wavepacket at time . We perform



../_images/math/19535649b870c7f042a21af576a87624636af2898f14582782ce0753cb8bf372a.png

steps of size .

Parameters:	tspan – <code>ndarray</code> consisting of end time at position 0, other positions are irrelevant.
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../_images/math/499a2ee48b33448e80b97af9df95508.png

`pre_propagate()`¶ Given the wavefunction at initial



../_images/math/1410bd3aa3d34373bc7de52c132b4fd6f154019a.png

time , perform some computations exactly once be-

fore running the ordinary time propagation and after each time simulation data was saved.

This method does not raise an exception but instead just does nothing and returns.

`propagate(tspan)[source]`¶ This method does nothing.

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