Some comments on the imaginary time step method applied to the Schroedinger equation on the spatial lattice.

Piotr Magierski, Aurel Bulgac
Numerical tests: Marcin Staszczak (undergraduate student)

The method

$$\left| \Psi_j^{(n+1)} \right\rangle = e^{-\lambda \hat{H}} \left| \psi_j^{(n)} \right\rangle, \quad j = 1, \dots, N$$

$$\left| \Psi_j^{(n+1)} \right\rangle \xrightarrow[\text{normalization}]{\text{orthogonalization}} \left| \psi_j^{(n+1)} \right\rangle$$

λ - imaginary time step

$$\hat{H} \left| \psi_j^{(n)} \right\rangle \xrightarrow{\ n \to \infty\ } E_j \left| \psi_j^{(n)} \right\rangle$$

Problem I

$$e^{-\lambda \hat{H}} = \dots$$

Problem II

method of *orthogonalization*

Problem III

errors of discretization

$$e^{-\lambda \hat{H}} = 1 + \sum_{i=1}^{n} \frac{(-\lambda)^i}{i!} \hat{H}^i + O(\lambda^{n+1})$$

Usually used for n=1
Drawbacks: - slow convergence.
- divergent for too large imaginary time step.
- numerically costly for n>1.

Alternative: we look for the expansion of $\exp(-\lambda \hat{H}) = \exp(-\lambda(\hat{T} + \hat{V}))$ in the form of product of exponents.

$$e^{-\lambda \hat{H}} = e^{-\frac{\lambda}{2}\hat{T}} e^{-\lambda \hat{V}} e^{-\frac{\lambda}{2}\hat{T}} + O(\lambda^3),$$ - second order method

$$e^{-\lambda \hat{H}} = e^{-\frac{\lambda}{6}\hat{V}} e^{-\frac{\lambda}{2}\hat{T}} e^{-\frac{2\lambda}{3}\tilde{V}} e^{-\frac{\lambda}{2}\hat{T}} e^{-\frac{\lambda}{6}\hat{V}} + O(\lambda^5),$$ - fourth order method

M. Aichinger
E. Krotscheck,
Comput. Mater. Sci.
34, 188 (2005)

$$\tilde{V} = \hat{V} + \frac{1}{48} \lambda^2 [\hat{V},[\hat{T},\hat{V}]]$$ - dominant term is local in space if $\hat{V}$ is local.

The above expansions are particularly useful if the Hamiltonian can be expressed as a sum of terms either local in the coordinate space (potential), or in the momentum space (kinetic energy).
In such a case one is adviced to use Fast Fourier Transform algorithm during the evolution of the wave function.

$$e^{-\lambda \hat{T}} \psi(\vec{p}) = e^{-\lambda \frac{p^2}{2m}} \psi(\vec{p})$$

$$e^{-\lambda \hat{V}} \psi(\vec{r}) = e^{-\lambda V(\vec{r})} \psi(\vec{r})$$

FFT

REAL SPACE ⟺ **MOMENTUM SPACE**

Advantages:
- Much faster convergence (**order of magnitude** difference between the first order and the second order method).
- The methods **do not diverge** even for large time steps.
- The cost of **FFT** instead of matrix multiplication.
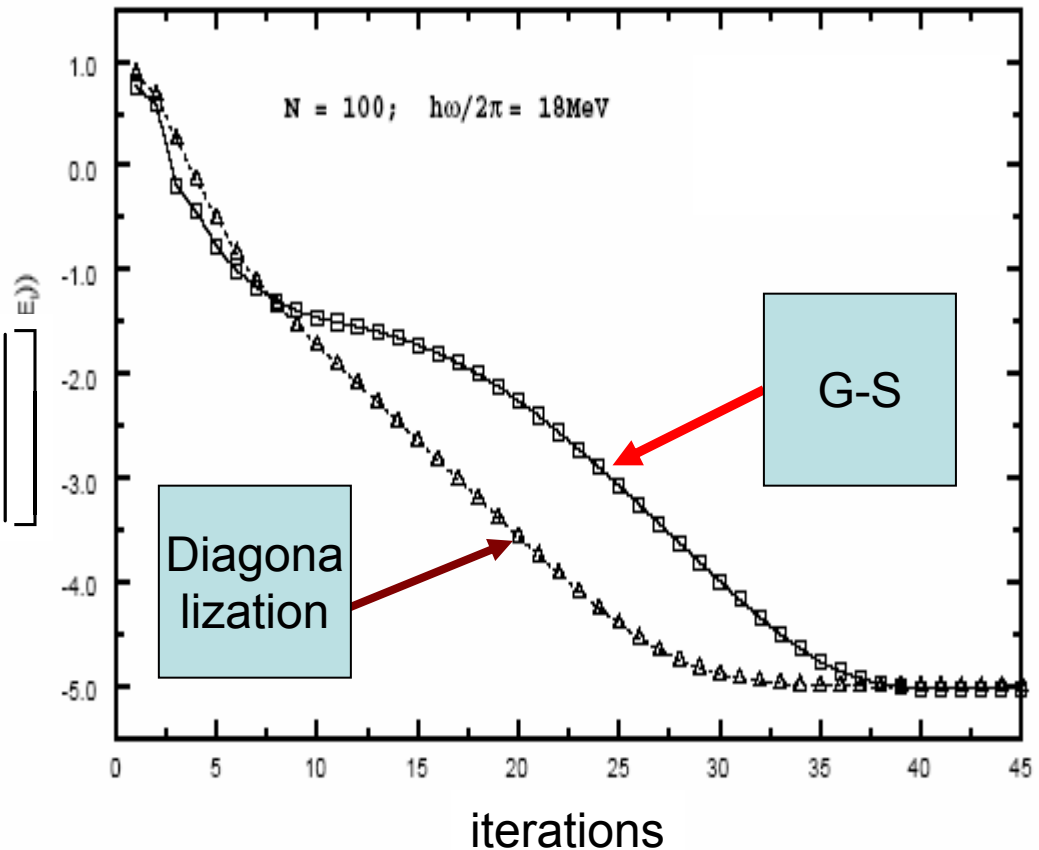
Problem II

<u>Orthogonalization:</u>

-Gram-Schmidt method (G-S)

-Diagonalization of the norm matrix

$$M_{ij} = \langle \Psi_i^{(n+1)} | \Psi_j^{(n+1)} \rangle,$$

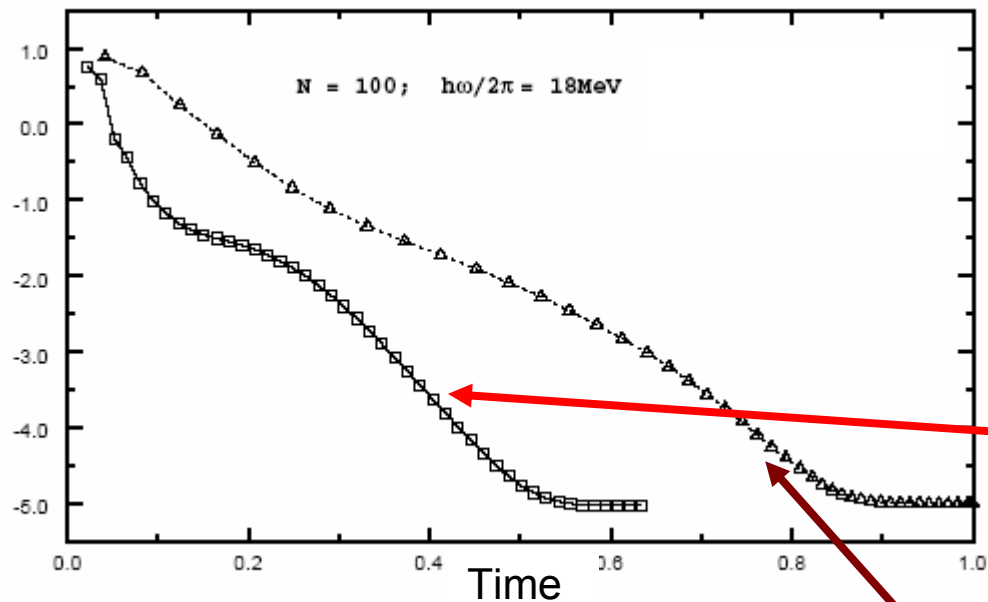Details of calculations:
-Lowest 100 states of 3-dim
 harmonic oscillator.
- Very bad first approx. for
  the w.f.: delta functions in
  the corner of the box.

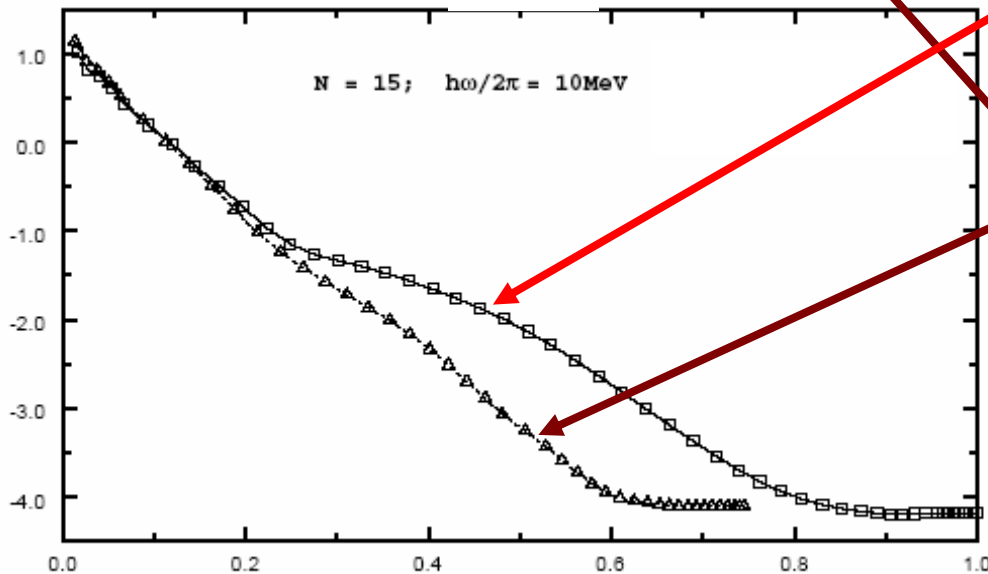$$Log\left[\frac{1}{N} \sum_i \left| \frac{E_i^{exact} - E_i}{E_i^{exact}} \right| \right]$$

N = 100;   hω/2π = 18MeV

G-S

Diagona
lization

iterations

$$Log\left[\frac{1}{N}\sum_i\left|\frac{E_i^{exact}-E_i}{E_i^{exact}}\right|\right]$$

N = 100;   ħω/2π = 18MeV

Time

N = 15;   ħω/2π = 10MeV

G-S

Diagonalization

$$Log\left[\frac{1}{N}\sum_i\left|\frac{E_i^{exact}-E_i}{E_i^{exact}}\right|\right]$$

It is adviced to use the G-S method at the beginning of the evolution when the number of evolved states is still large. When the number of evolved states decreases one has to apply diagonalization of the norm.
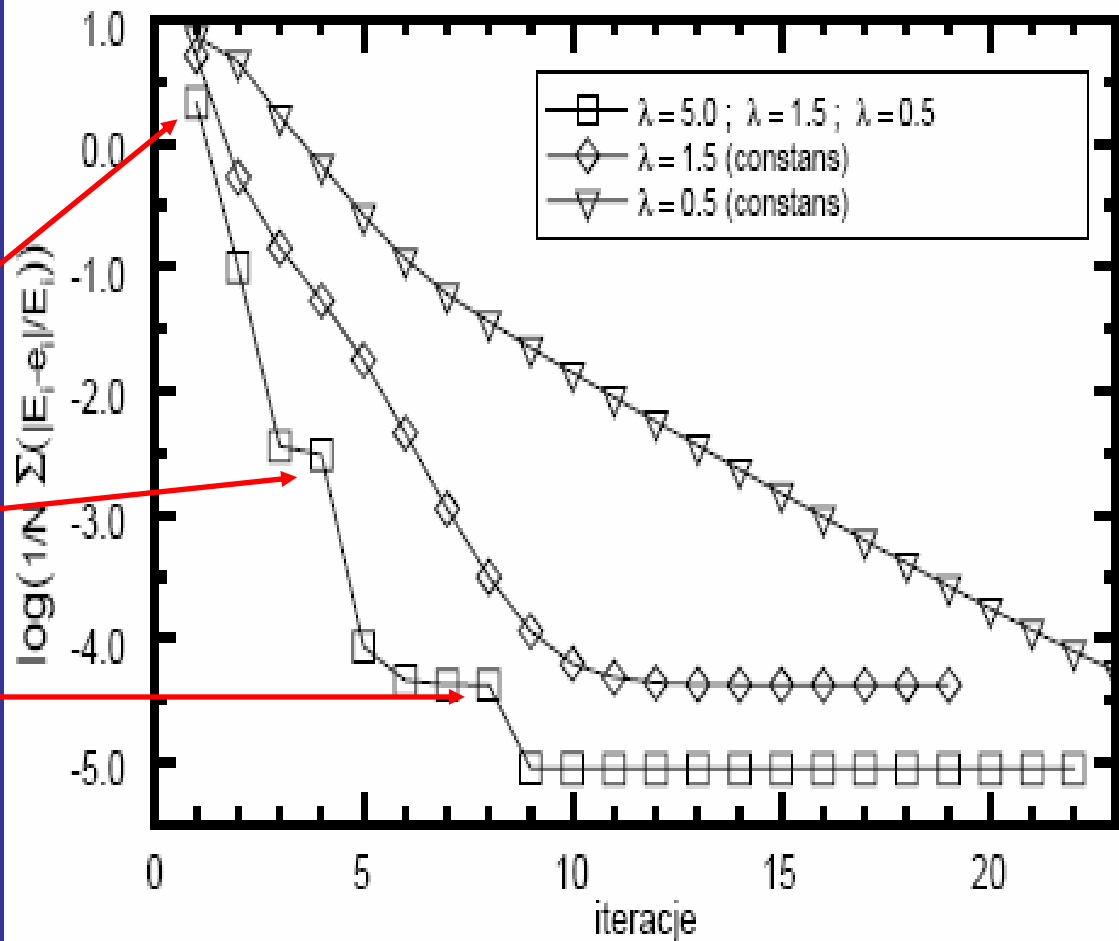
-One may vary imaginary time step during calculations:
 starting with the large time step and decreasing it subsequently

λ is in units of $\left(\dfrac{\hbar^2}{2md^2}\right)^{-1}$,

where d is the lattice constant.

$\lambda = 5.0$

$\lambda = 1.5$

$\lambda = 0.5$

Legend:
- $\lambda = 5.0$; $\lambda = 1.5$; $\lambda = 0.5$
- $\lambda = 1.5$ (constans)
- $\lambda = 0.5$ (constans)

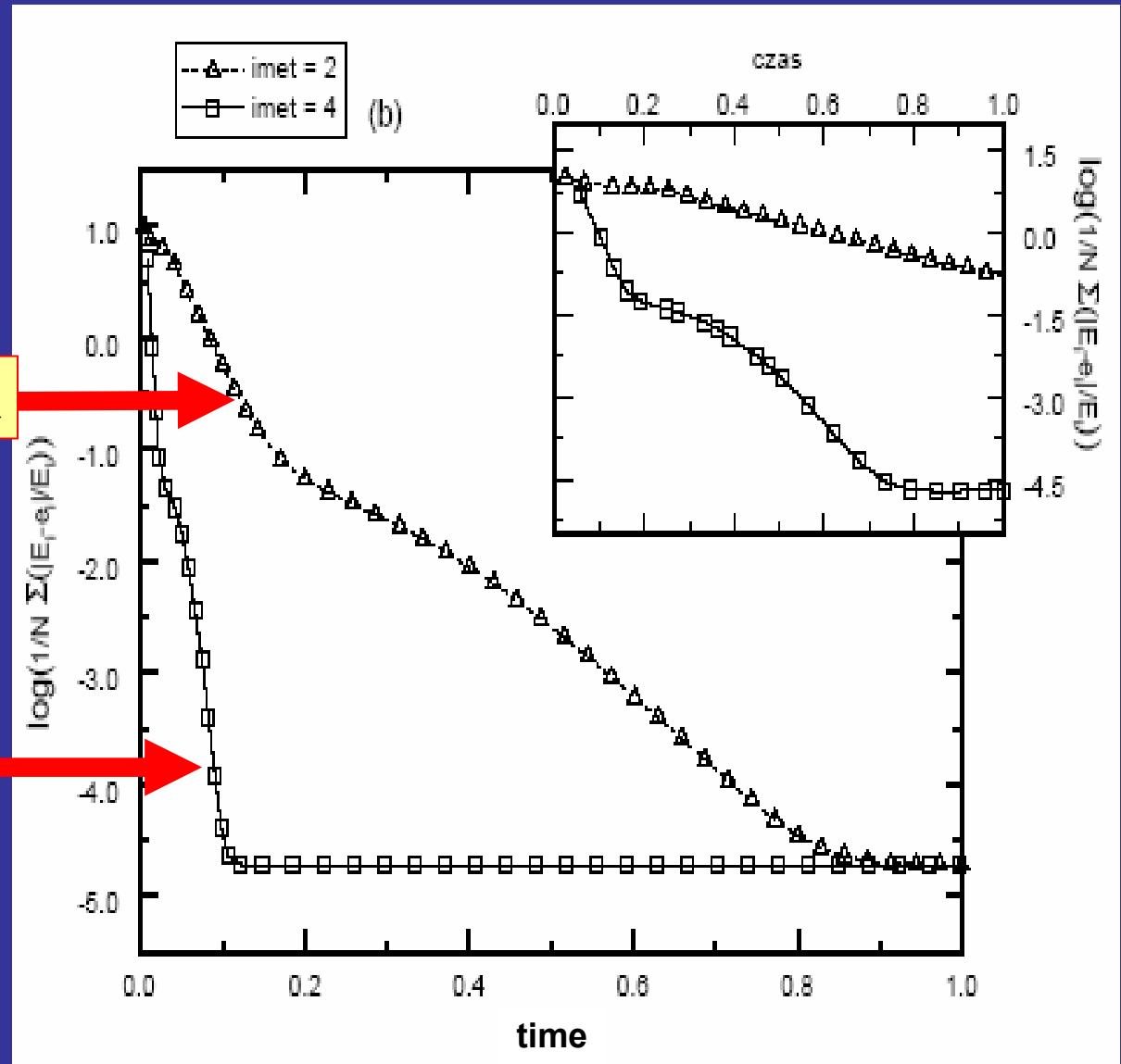y-axis: $\log(1/N \sum(|E_r - e_i|/E_i))$

x-axis: iteracje

Varying the imaginary time step one can reach faster convergence!

Comparison between the second and the fourth order method

second order method

fourth order method

errors of discretization

$$Potential : V(\vec{r}) = \frac{V_1}{1 + e^{-R_1/a_1} \cosh(r_+ / a_1)} + \frac{V_2}{1 + e^{-R_2/a_2} \cosh(r_- / a_2)}$$

$$r_+ = \sqrt{x^2 + y^2 + (z + \zeta)^2}, r_- = \sqrt{x^2 + y^2 + (z - \zeta)^2}$$
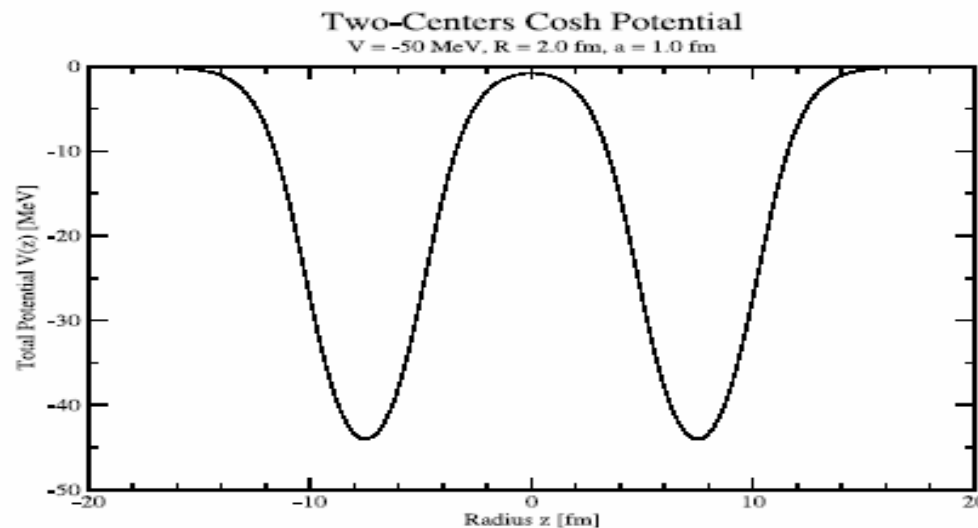
$$V_1 = V_2 = -50 MeV$$

$$R_1 = R_2 = 2 fm$$

$$a_1 = a_2 = 1 fm$$

$$\zeta = 7.5 fm$$

Size of the box L=40fm

Two-Centers Cosh Potential
V = -50 MeV, R = 2.0 fm, a = 1.0 fm

State	Energies (Hamiltonian)	$<r^2>^{(1/2)}$	Log(error)
1	-22.154200	7.810782	-18.232979
2	-22.154064	7.810914	-17.475285
3	-9.101107	8.113153	-16.849039
4	-9.092759	8.122956	-16.555068
5	-9.092759	8.122956	-16.555068
6	-9.091346	8.124427	-17.180201
7	-9.091346	8.124427	-17.180201
8	-9.085579	8.132505	-17.311714
9	-1.657758	9.214863	-18.245006
10	-1.442607	9.531731	-16.997455

Evolution   =   76.08755   %
Diagonalization =   23.42908   %

State	Energies (Hamiltonian)	$<r^2>^{(1/2)}$	Log(error)
1	-22.154200	7.810777	-25.216463
2	-22.154064	7.810910	-16.660222
3	-9.101116	8.113149	-19.933659
4	-9.092750	8.122955	-18.104582
5	-9.092750	8.122955	-18.104582
6	-9.091337	8.124426	-18.314712
7	-9.091337	8.124426	-18.314712
8	-9.085588	8.132502	-19.871574
9	-1.657762	9.214920	-18.775086
10	-1.442613	9.531756	-19.942593

Evolution   =   72.09885   %
Diagonalization =   27.70120   %

State	Energies (Hamiltonian)	$<r^2>^{(1/2)}$	Log(error)
1	-22.154200	7.810775	-16.994214
2	-22.154064	7.810907	-16.493751
3	-9.101116	8.113147	-18.013862
4	-9.092750	8.122954	-16.789668
5	-9.092750	8.122954	-16.789668
6	-9.091337	8.124425	-17.115993
7	-9.091337	8.124425	-17.115993
8	-9.085588	8.132501	-17.411483
9	-1.657762	9.214822	-16.551662
10	-1.442613	9.531734	-19.358748

Evolution   =   90.60242   %
Diagonalization =   7.823270   %

$$\int \rho\, d^3r = 10.000000000 \qquad 10.000000000 \qquad 10.000000000$$

$$\int \rho^2\, d^3r = 0.177376948 \qquad 0.177379729 \qquad 0.177381333$$

$$\int \rho^3\, d^3r = 0.005339013 \qquad 0.005339294 \qquad 0.005339416$$

Relative accuracy at d=0.8fm : $\quad 2 \times 10^{-5}$

Comparison between methods: imaginary time step, wavelet, h.o. basis

d=0.8fm

N	State (2-cosh)	Wavelet	HO basis
1	1/2 (+)	-22.1542	-22.0963
2	1/2 (-)	-22.1540	-22.0961
3	1/2 (+)	-9.1011	-9.0200
4	1/2 (-)	-9.0927	-9.0121
5	3/2 (-)	-9.0926	-9.0121
6	1/2 (+)	-9.0913	-9.0107
7	3/2 (+)	-9.0912	-9.0107
8	1/2 (-)	-9.0857	-9.0051
9	1/2 (+)	-1.6541	-1.6008
10	1/2 (-)	-1.4472	-1.3944

State	Energies (Hamiltonian)	$\langle r^2 \rangle^{(1/2)}$	Log(error)
1	-22.154200	7.810777	-25.216463
2	-22.154064	7.810910	-16.660222
3	-9.101116	8.113149	-19.933659
4	-9.092750	8.122955	-18.104582
5	-9.092750	8.122955	-18.104582
6	-9.091337	8.124426	-18.314712
7	-9.091337	8.124426	-18.314712
8	-9.085588	8.132502	-19.871574
9	-1.657762	9.214920	-18.775086
10	-1.442613	9.531756	-19.942593

Evolution   = 72.09885   %
Diagonalization =   27.70120   %

Summary

- The scheme is fast comparing to the first order expansion (by an order of magnitude!)

- It is always convergent (no matter how large is time step).

- It is simple. The code of 500 lines (fortan 90) solves the eigenproblem for a potential of arbitary shape. Shape of the potential does not influence the accuracy (up to discretization errors).

- The method is easily parallelizable.

- Spin-orbit:

$$e^{-\lambda\hat{H}} \approx e^{-\frac{\lambda}{2}\hat{T}} e^{-\frac{\lambda}{2}\hat{V}} \left(1 - \lambda \nabla V_{so}(\vec{r},\vec{p})\bullet\vec{S} + \frac{\lambda^2}{2}\left(\nabla V_{so}(\vec{r},\vec{p})\bullet\vec{S} \right)^2 \right) e^{-\frac{\lambda}{2}\hat{V}} e^{-\frac{\lambda}{2}\hat{T}}$$

- Possibility to include nonlocal potentials even in the fourth order method:

$$e^{-\lambda\hat{H}} \approx e^{-\frac{\lambda}{6}\hat{V}_{nloc}} e^{-\frac{\lambda}{2}\hat{H}_{loc}} e^{-\frac{2\lambda}{3}\tilde{V}_{nloc}} e^{-\frac{\lambda}{2}\hat{H}_{loc}} e^{-\frac{\lambda}{6}\hat{V}_{nloc}} ; \ \hat{H}_{loc} = \hat{T} + V(\vec{r})$$