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

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The method

\[
\begin{align*}
\left| \Psi_j^{(n+1)} \right\rangle &= e^{-\lambda \hat{H}} \left| \psi_j^{(n)} \right\rangle, \quad j = 1, \ldots, N \\
\left| \Psi_j^{(n+1)} \right\rangle &\xrightarrow{\text{orthogonalization}} \left| \psi_j^{(n+1)} \right\rangle \\
\lambda &- \text{imaginary time step}
\end{align*}
\]

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

Problem I

\[e^{-\lambda \hat{H}} = \ldots\]

Problem II

method of orthogonalization

Problem III

errors of discretization
Problem I

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

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.

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

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

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

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 advised to use Fast Fourier Transform algorithm during the evolution of the wave function.

\[
\begin{align*}
  e^{-\frac{\hat{V}}{\lambda}} \psi(\vec{r}) &= e^{-\lambda \frac{p^2}{2m}} \psi(\vec{p}) \\
  e^{-\frac{\hat{T}}{\lambda}} \psi(\vec{p}) &= e^{-\lambda V(\vec{r})} \psi(\vec{r})
\end{align*}
\]

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.
Orthogonalization:
- 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.

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

$N = 100; \quad \hbar \omega / 2\pi = 18 \text{ meV}$
It is advised 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.
Some advantages of the method:

- One may vary imaginary time step during calculations: starting with the large time step and decreasing it subsequently.

$\lambda$ is in units of $\left(\frac{\hbar^2}{2md^2}\right)^{-1}$, where $d$ is the lattice constant.

$\lambda = 5.0$
$\lambda = 1.5$
$\lambda = 0.5$

Varying the imaginary time step one can reach faster convergence!
Comparison between the second and the fourth order method
Potential: \( V(\vec{r}) = \frac{V_1}{1 + e^{\frac{-R_1}{a_1}} \cosh(r_+/a_1)} + \frac{V_2}{1 + e^{\frac{-R_2}{a_2}} \cosh(r_-/a_2)} \)

\[ r_+ = \sqrt{x^2 + y^2 + (z + \zeta)^2}, \quad r_- = \sqrt{x^2 + y^2 + (z - \zeta)^2} \]

\( V_1 = V_2 = -50 \text{ MeV} \)

\( R_1 = R_2 = 2 \text{ fm} \)

\( a_1 = a_2 = 1 \text{ fm} \)

\( \zeta = 7.5 \text{ fm} \)

Size of the box L=40 fm
d=1.0fm

<table>
<thead>
<tr>
<th>State</th>
<th>Energies (Hamiltonian)</th>
<th>(&lt;r^2&gt;^{1/2}\rangle)</th>
<th>Log(error)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>-22.154200</td>
<td>7.810782</td>
<td>-18.232979</td>
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<tr>
<td>2</td>
<td>-22.154064</td>
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<tr>
<td>6</td>
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<td>9</td>
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<td>-16.997455</td>
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</tbody>
</table>

\[
\int \rho d^3r = 10.000000000
\]
\[
\int \rho^2 d^3r = 0.177376948
\]
\[
\int \rho^3 d^3r = 0.005339013
\]

Relative accuracy at d=0.8fm : \(2 \times 10^{-5}\)
Comparison between methods: imaginary time step, wavelet, h.o. basis

d=0.8fm

<table>
<thead>
<tr>
<th>N</th>
<th>State (2-cosh)</th>
<th>Wavelet</th>
<th>HO basis</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1/2 (+)</td>
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<td>1/2 (-)</td>
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<td>-22.0961</td>
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<tr>
<td>3</td>
<td>1/2 (+)</td>
<td>-9.1011</td>
<td>-9.0200</td>
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<td>4</td>
<td>1/2 (-)</td>
<td>-9.0927</td>
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<tr>
<td>5</td>
<td>3/2 (-)</td>
<td>-9.0926</td>
<td>-9.0121</td>
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<td>10</td>
<td>1/2 (-)</td>
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<td>-1.3944</td>
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</tbody>
</table>

State Energies \langle r^2 \rangle ^{1/2} \text{Log(error)}

(Hamiltonian)

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 %
Procedure

Imaginary time step
Time step is varied (decreasing)

Preorthogonalization
G-S method is used to decouple space of already converged states

G-S method
(N - large)

Diagonalization of the norm matrix
(N - smaller)
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 arbitrary shape. Shape of the potential does not influence the accuracy (up to discretization errors).

- The method is easily parallelizable.

- Spin-orbit:

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

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

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