Split-Operator Fourier Transform Algorithm

Often, we are interested in the time evolution of system. Especially in quantum mechanics it is not trivial to study the time evolution of a system. In the following, I'll sketch the full derivation of the algorithm which I outlined in the video.

As in the video, we start with the time dependent SCHRÖDINGER equation, which reads

$$\frac{\partial \left|\Psi\left(t\right)\right\rangle}{\partial t} = \hat{\mathcal{H}} \left|\Psi\left(t\right)\right\rangle . \tag{1}$$

Here we used the DIRAC notation. If you're not familiar with this, I encourage you to read the corresponding wikipedia article (`https://en.wikipedia.org/wiki/Bra%E2%80%93ket_notation`, in a nutshell it is some way to write down inner products) and the HAMILTONian $\hat{\mathcal{H}}$ which is the operator that gives us the energy and which is built out of two parts

$$\hat{\mathcal{H}} = \hat{\mathcal{T}} + \hat{\mathcal{V}}, \tag{2}$$

namely one for the kinetic energy ($\hat{\mathcal{T}}$) and another one for the potential energy ($\hat{\mathcal{V}}$). Note, that we did not specify a basis yet. We represent the state of the system in a complete abstract way with the ket $\left|\Psi\left(t\right)\right\rangle$.

If we assume that our HAMILONian is time independent, equation 1 is easy to integrate and gives rise to the following solution

$$\left|\Psi\left(t\right)\right\rangle = \exp\left(-\frac{\mathrm{i}\hat{\mathcal{H}}}{\hbar}\right)\left|\Psi\left(0\right)\right\rangle , \tag{3}$$

which tells us that we arrive at the system at time t by applying the exponential of the HAMILONian onto the initial state at $t = 0$. We call this exponential operator which propagates our system from $t = 0$ to t propagator.

Unfortunately, we have no idea what the result of the action of this propagator onto your system yields for some arbitrary HAMILTONian.

In the following, we will use to approximation to get to an *controllable* approximation. I.e. an approximation where we know how large the error is and where we introduce it. We do this with two steps:

1. We use the time composition property to write propagation as a sequence of small time steps

2. We introduce the trotter approximation, where we know how large the error with different operator split-ups is.

To do this, we write your equation for the propagation (eq. 3) in a less abstract way, i.e. we chose the coordinate representation. To to this we project our state $|\Psi(t)\rangle$ onto the coordinate basis x_t:

$$\begin{aligned} \langle x_0 \,|\, \Psi(t)\rangle = & \left\langle x_t \left| \exp\left(-\frac{\mathrm{i}\hat{\mathcal{H}}}{\hbar}\right) \right| \Psi(x_0) \right\rangle \\ = & \int \mathrm{d}x_0 \underbrace{\left\langle x_t \left| \exp\left(-\frac{\mathrm{i}\hat{\mathcal{H}}}{\hbar}\right) \right| x_0 \right\rangle}_{K(x_t,x_0)} \underbrace{\langle x_0 \,|\, \Psi(0)\rangle}_{\Psi(x_0;0)} \end{aligned} \tag{4}$$

Where we introduced a resolution of the identity

$$\int \mathrm{d}x_0 \, |x_0\rangle \langle x_0| = 1 \tag{5}$$

to get an expression for the propagator in the coordinate representation, $K(x_t, x_0)$, which we can identically rewrite as follows

$$\begin{aligned} K(x_t, x_0) = & \left\langle x_t \left| \exp\left(-\frac{\mathrm{i}\hat{\mathcal{H}}t}{\hbar}\right) \right| x_0 \right\rangle \\ = & \left\langle x_{N+1} \left| \exp\left(-\frac{\mathrm{i}\hat{\mathcal{H}}}{\hbar}\frac{t}{N}\right) \exp\left(-\frac{\mathrm{i}\hat{\mathcal{H}}}{\hbar}\frac{t}{N}\right) \cdots \exp\left(-\frac{\mathrm{i}\hat{\mathcal{H}}}{\hbar}\frac{t}{N}\right) \right| x_0 \right\rangle. \end{aligned} \tag{6}$$

We can now introduce a resolution of the identity (eq. 5) for each step:

$$\begin{aligned} K(x_t, x_0) = & \int \mathrm{d}x_N \cdots \mathrm{d}x_1 \left\langle x_{N+1} \left| \exp\left(-\frac{\mathrm{i}\hat{\mathcal{H}}}{\hbar}\frac{t}{N}\right) \right| x_N \right\rangle \\ & \cdot \left\langle x_N \left| \exp\left(-\frac{\mathrm{i}\hat{\mathcal{H}}}{\hbar}\frac{t}{N}\right) \right| x_{N-1} \right\rangle \\ & \cdots \left\langle x_1 \left| \exp\left(-\frac{\mathrm{i}\hat{\mathcal{H}}}{\hbar}\frac{t}{N}\right) \right| x_0 \right\rangle. \end{aligned} \tag{7}$$

We can use this knowledge in eq. 4:

$$\begin{aligned}
\left\langle x_{N+1} \left| \exp\left(-\frac{\mathrm{i}\hat{\mathcal{H}}}{\hbar}\frac{t}{N}\right) \right| \Psi(0) \right\rangle &= \Psi(x,t) \\
= \int \mathrm{d}x_N \mathrm{d}x_{N-1} \cdots \mathrm{d}x_1 \left\langle x_{N+1} \left| \exp\left(-\frac{\mathrm{i}\hat{\mathcal{H}}}{\hbar}\frac{t}{N}\right) \right| x_N \right\rangle & \\
\cdot \left\langle x_N \left| \exp\left(-\frac{\mathrm{i}\hat{\mathcal{H}}}{\hbar}\frac{t}{N}\right) \right| x_{N-1} \right\rangle & \\
\cdots \left\langle x_1 \left| \exp\left(-\frac{\mathrm{i}\hat{\mathcal{H}}}{\hbar}\frac{t}{N}\right) \right| x_0 \right\rangle \Psi\left(x_0, 0\right). &
\end{aligned} \tag{8}$$

Especially if we just look at one step

$$\int \mathrm{d}x_1 \left\langle x_1 \left| \exp\left(-\frac{\mathrm{i}\hat{\mathcal{H}}}{\hbar}\frac{t}{N}\right) \right| x_0 \right\rangle \Psi\left(x_0\right) = \Psi\left(x_1, \epsilon\right), \tag{9}$$

we notice that this gives rise to a time-stepping algorithm. If we introduce the time-step

$$\frac{t}{N} = \epsilon, \tag{10}$$

we can write the single step as

$$\langle x_1 \,|\, \Psi\left(\epsilon\right)\rangle = \Psi\left(x_1, \epsilon\right) = \int \mathrm{d}x_0 \left\langle x_1 \left| \exp\left(-\frac{\mathrm{i}\hat{\mathcal{H}}}{\hbar}\epsilon\right) \right| x_0 \right\rangle \Psi\left(x_0, 0\right). \tag{11}$$

This was the first step of our journey to the algorithm. Next, we are going to introduce the Trotter split-up formula, which tells us that for infinitesimally small time steps ϵ we can write

$$\exp\left[\mathrm{i}\left(\hat{\mathcal{H}}_1 + \hat{\mathcal{H}}_2\right)\right] = \lim_{N\to\infty} \left[\exp\left(\mathrm{i}\hat{\mathcal{H}}_2\frac{t}{2N}\right) \exp\left(\mathrm{i}\hat{\mathcal{H}}_1\frac{t}{N}\right) \exp\left(\mathrm{i}\hat{\mathcal{H}}_2\frac{t}{2N}\right)\right]^N, \tag{12}$$

where in our case $\hat{\mathcal{H}}_1 = \hat{\mathcal{T}}$ and $\hat{\mathcal{H}}_2 = \hat{\mathcal{V}}$.

If we no assume a less abstract form of our Hamiltonian, e.g.

$$\hat{\mathcal{H}} = \hat{\mathcal{T}} + \hat{\mathcal{V}}\left(\hat{x}\right) = \frac{\hat{p}^2}{2m} + \hat{\mathcal{V}}\left(\hat{x}\right) \tag{13}$$

we can use the symmetrical Trotter split up to write

$$
\begin{aligned}
&\left\langle x_1 \left| \exp\left[-\frac{\mathrm{i}}{\hbar}\left(\frac{\hat{p}^2}{2m}+V(\hat{x})\right)\epsilon\right] \right| x_0 \right\rangle \\
&\approx \left\langle x_1 \left| \exp\left[-\frac{\mathrm{i}}{\hbar}V(\hat{x})\frac{\epsilon}{2}\right] \exp\left[-\frac{\mathrm{i}}{\hbar}\left(\frac{\hat{p}^2}{2m}\right)\epsilon\right] \exp\left[-\frac{\mathrm{i}}{\hbar}V(\hat{x})\frac{\epsilon}{2}\right] \right| x_0 \right\rangle \\
&= \exp\left[-\frac{\mathrm{i}}{\hbar}V(x_1)\frac{\epsilon}{2}\right] \left\langle x_1 \left| \exp\left[-\frac{\mathrm{i}}{\hbar}\left(\frac{\hat{p}^2}{2m}\right)\epsilon\right] \right| x_0 \right\rangle \exp\left[-\frac{\mathrm{i}}{\hbar}V(x_0)\frac{\epsilon}{2}\right] \\
&= \exp\left[-\frac{\mathrm{i}}{\hbar}V(x_1)\frac{\epsilon}{2}\right] \int \mathrm{d}p \left\langle x_1 \left| \exp\left[-\frac{\mathrm{i}}{\hbar}\left(\frac{\hat{p}^2}{2m}\right)\epsilon\right] \right| p \right\rangle \langle p \mid x_0 \rangle \exp\left[-\frac{\mathrm{i}}{\hbar}V(x_0)\frac{\epsilon}{2}\right]
\end{aligned}
\tag{14}
$$

Note that we multiple times introduce the resolution of the identity (e.g. it is not explicitely written in line 2 for the projection of the second exponential on x_0).

Now, it is useful to know, what $\langle p \mid x_0 \rangle$ is, following argument shall rationalize the well-known result:

$$
\begin{aligned}
\hat{p}\,|p\rangle &= p\,|p\rangle && (15)\\
\langle x \mid \hat{p} \mid p \rangle &= p \langle x \mid p \rangle && (16)\\
-\mathrm{i}\frac{\partial}{\partial x}\langle x \mid p \rangle &= \frac{p}{\hbar}\langle x \mid p \rangle && (17)
\end{aligned}
$$

since

$$
\hat{p} = -\mathrm{i}\hbar\frac{\partial}{\partial x}, \tag{18}
$$

solving this differential equation for $\langle x \mid p \rangle$ yields

$$
\langle x \mid p \rangle = \frac{1}{\sqrt{2\pi\hbar}} \exp\left(\frac{\mathrm{i}}{\hbar}px\right) \tag{19}
$$

Thus, we can write

$$
\begin{aligned}
&\left\langle x_1 \left| \exp\left[-\frac{\mathrm{i}}{\hbar}\left(\frac{\hat{p}^2}{2m}+V(\hat{x})\right)\epsilon\right] \right| x_0 \right\rangle = \\
&\exp\left[-\frac{\mathrm{i}}{\hbar}V(x_1)\frac{\epsilon}{2}\right] \int \frac{\mathrm{d}p}{2\pi\hbar} \exp\left(\frac{\mathrm{i}}{\hbar}px_1\right) \exp\left(-\frac{\mathrm{i}}{\hbar}\frac{p^2}{2m}\epsilon\right) \\
&\qquad \cdot \exp\left(-\frac{\mathrm{i}}{\hbar}px_0\right) \exp\left[-\frac{\mathrm{i}}{\hbar}V(x_0)\frac{\epsilon}{2}\right]
\end{aligned}
\tag{20}
$$

Note that *via* the projections we transformed the operators $\hat{x}$ and $\hat{p}$ into c-numbers.

Now, let's use this result in eq. 11:

$$\Psi(x_1,\epsilon) = \exp\left[-\frac{\mathrm{i}}{\hbar}V(x_1)\frac{\epsilon}{2}\right]\int\frac{\mathrm{d}p}{\sqrt{2\pi\hbar}}\exp\left(\frac{\mathrm{i}}{\hbar}px_1\right)\exp\left(-\frac{\mathrm{i}}{\hbar}\frac{p^2}{2m}\epsilon\right)$$
$$\underbrace{\cdot\int\frac{\mathrm{d}x_0}{\sqrt{2\pi\hbar}}\exp\left(-\frac{\mathrm{i}}{\hbar}px_0\right)\underbrace{\exp\left[-\frac{\mathrm{i}}{\hbar}V(x_0)\frac{\epsilon}{2}\right]\Psi(x_0,0)}_{\Phi_{\frac{\epsilon}{2}}(x_0)}}_{\tilde{\Phi}_{\frac{\epsilon}{2}}(p)} \tag{21}$$

Continue our FOURIER transform game

$$\Psi(x_1,\epsilon) = \exp\left[-\frac{\mathrm{i}}{\hbar}V(x_1)\frac{\epsilon}{2}\right]\underbrace{\int\frac{\mathrm{d}p}{\sqrt{2\pi\hbar}}\exp\left(\frac{\mathrm{i}}{\hbar}px_1\right)\underbrace{\exp\left(-\frac{\mathrm{i}}{\hbar}\frac{p^2}{2m}\epsilon\right)\tilde{\Phi}_{\frac{\epsilon}{2}}(p)}_{\tilde{\Phi}_\epsilon(p)}}_{\Phi_\epsilon(x_1)} \tag{22}$$
$$= \exp\left[-\frac{\mathrm{i}}{\hbar}V(x_1)\frac{\epsilon}{2}\right]\Phi_\epsilon(x_1)$$

Iterate N times to get $\Psi(x_{N+1}), t = (N+1)\epsilon$.

In summary we start in x-representation, propagate a half-step of our potential-propagator, transform to p-representation apply there our kinetic energy operator and transform then back to x-representation where we conveniently can apply our potential propagator.

Numerically, this is implemented *via* a discrete FOURIER transform (integration over a grid). Doing FOURIER transforms is computationally cheap, it scales with $N \lg N$, where N is the number of grid points. But, if one goes to multiply dimensions N^n, where n is the number of dimensions, one hits the exponential wall. Nevertheless, the algorithm is used as benchmark for other approximations – as we exactly now how large the error of our trotter approximation is (i.e. it depends on the commutator).

The calculation can be made a bit less expensive with adaptive grids or soft grids.

I mentioned that this technique can also be used to derive algorithms for molecular dynamics simulation. In fact, this can be done starting with the LIOUVILLE operator as e.g. shown in *J. Chem. Phys.* **1992**, *97*, 1990-2001.

Recommended literature to the sections of the video

- free wave packet: `https://www.colorado.edu/physics/phys2170/phys2170_sp07/downloads/Gaussian.pdf`
- spreading of wave packets: Quantum Mechanics: Concepts and Applications by Nouredine Zettili, Chapter 1 (Wiley, 2009).
- SOFT algorithm: Time-Dependent Quantum Molecular Dynamics by Broeckhove and Lathouwers (Springer, 1992).