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Quantum simulators - Exercise sheet No. 2

a) To find the potential that correspond to the following wave functions as ground state we suppose the Hamiltonian:

$$\hat{H} = \frac{\vec{\hat{P}}^2}{2m} + V(r)$$

and it's respective schrödinger equation to ground state

$$\hat{H} |\psi_0\rangle = E_0 |\psi\rangle$$

and in coordinates space

$$\int d^3x' \langle x | \hat{H} | x' \rangle \langle x' | \psi_0 \rangle = E_0 \langle x | \psi_0 \rangle$$

$$\left[-\frac{\hbar^2}{2m} \vec{\nabla}^2 + V(r) \right] \psi_0(r) = E_0 \psi_0(r)$$

Taking into account that since the wave function is in term of spherical coordinates the Hamiltonian also be. so we replace for the first wavefunction and calculate the potential

$$\psi_0(r) = e^{-\alpha r^2}$$

$$-\frac{\hbar^2}{2m} \vec{\nabla}^2 (e^{-\alpha r^2}) + V(r) e^{-\alpha r^2} = E_0 e^{-\alpha r^2}$$

The Laplacian in spherical coordinates will be

$$-\frac{\hbar^2}{2m} \vec{\nabla}^2 (e^{-\alpha r^2}) = -\frac{\hbar^2}{2m} \frac{1}{r^2} \frac{\partial}{\partial r} \left[r^2 \frac{\partial}{\partial r} \left(e^{-\alpha r^2} \right) \right]$$

$$= \frac{-\hbar^2}{2m} \frac{1}{r^2} \frac{\partial}{\partial r} \left[-2\alpha r^3 e^{-\alpha r^2} \right]$$

$$= \frac{\alpha \hbar^2}{m} \frac{1}{r^2} \left(3 r^2 e^{-\alpha r^2} - 2\alpha r^4 e^{-\alpha r^2} \right)$$

$$= \frac{\alpha \hbar^2}{m} e^{-\alpha r^2} \left(3 - 2\alpha r^2 \right)$$

Then

$$\frac{\alpha\hbar^2}{m} \cancel{e^{-\alpha r^2}} (3 - 2\alpha r^2) + V(r)\cancel{e^{-\alpha r^2}} = E_0 \cancel{e^{-\alpha r^2}}$$

$$\boxed{V(r) = \frac{2\alpha^2\hbar^2}{m} r^2 + E_0 - \frac{3\alpha\hbar^2}{m}}$$

In order to $V(r)$ be physically reasonable E_0 must be the minimal energy of the system, so since the potential and the kinetic energy are quadratic, always will be positive and growing therefore the minimom is when there is neither kinetic nor potental energy then the resulting energy only will come to the shifts i.e E_0 & $-\frac{3\alpha\hbar^2}{m}$ and as E_T must be positive $E_0 \geq \frac{3\alpha\hbar^2}{m}$

b) In this case

$$\psi_0(r) = e^{-\alpha r}$$

so doing the same process as in the previous point

$$\left[-\frac{\hbar^2}{2m}\vec{\nabla}^2 + V(r)\right] e^{-\alpha r} = E_0 e^{-\alpha r}$$

$$-\frac{\hbar^2}{2m}\vec{\nabla}^2(e^{-\alpha r}) + V(r)\, e^{-\alpha r} = E_0 e^{-\alpha r}$$

Then

$$-\frac{\hbar^2}{2m}\vec{\nabla}^2(e^{-\alpha r}) = -\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{\partial}{\partial r}\left[r^2\frac{\partial}{\partial r}\left(e^{-\alpha r}\right)\right]$$

$$= -\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{\partial}{\partial r}\left[-\alpha r^2 e^{-\alpha r}\right]$$

$$= \frac{\alpha\hbar^2}{2m}\frac{1}{r^2}\left(2r e^{-\alpha r} - \alpha r^2 e^{-\alpha r}\right)$$

$$= \frac{\alpha\hbar^2}{2m} e^{-\alpha r}\left(\frac{2}{r} - \alpha\right)$$

$$\frac{\alpha\hbar^2}{2m}\cancel{e^{-\alpha r}}\left(\frac{2}{r}-\alpha\right)+V(r)\cancel{e^{-\alpha r}}=E_0\cancel{e^{-\alpha r}}$$

$$V(r)=-\frac{\alpha\hbar^2}{m}\frac{1}{r}+E_0+\frac{\alpha^2\hbar^2}{2m}$$

Now for this potential the conditions will be, $r>0$ i.e. $r\neq 0$ since r for definition is $r\geqslant 0$ and $E_0\sim\frac{\alpha\hbar^2}{m}$ for E_T to be positive.

b) And finally

$$\psi_0(x)=\frac{1}{\cosh(x)}$$ in this case is 1D so $\vec{\nabla}^2=\frac{d^2}{dx^2}$

Then

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(x)\right]\frac{1}{\cosh(x)}=E_0\frac{1}{\cosh(x)}$$

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\left(\frac{1}{\cosh(x)}\right)+\frac{V(x)}{\cosh(x)}=\frac{E_0}{\cosh(x)}$$

$$-\frac{\hbar^2}{2m}\frac{d}{dx}\left(-\frac{\operatorname{senh}(x)}{\cosh^2(x)}\right)+\frac{V(x)}{\cosh(x)}=\frac{E_0}{\cosh(x)}$$

$$\frac{\hbar^2}{2m}\left(\frac{\cosh^3(x)-2\cosh(x)\operatorname{senh}^2(x)}{\cosh^3(x)}\right)+V(x)=E_0$$

$$\frac{\hbar^2}{2m}\left(1-2\tanh^2(x)\right)+V(x)=E_0$$

$$V(x)=\frac{\hbar^2}{2m}\left(2\tanh^2(x)-1\right)+E_0$$

Now in this case all values of x are allow and the minimum is for $x=0$ and that value is positive, so E_0 just must be $E_0>0$ in order to the total energy be positive.

2) Given the hamiltonian

$$\hat{H} = \hat{\sigma}_z + \Gamma \hat{\sigma}_x := \begin{pmatrix} 1 & \Gamma \\ \Gamma & -1 \end{pmatrix}$$

To solve the exact dynamic, we calculate the time-evolution operator with the spectral decomposition

$$\hat{U}(t,0) = e^{-\frac{i}{\hbar}\hat{H}t} = \hat{R}^{+} e^{-\frac{i}{\hbar}\hat{D}t}\hat{R}$$

where $\hat{R}$ is the eigenvectors matrix and $\hat{D}$ the eigenenergies matrix of $\hat{H}$
Then we diagonalize the Hamiltonian in the usual form

$$\det(\hat{H} - \lambda \hat{1}) = 0$$

$$\begin{vmatrix} 1-\lambda & \Gamma \\ \Gamma & -(1+\lambda) \end{vmatrix} = 0 \longrightarrow 1 - \lambda^2 + \Gamma^2 = 0$$

$$\lambda = \pm\sqrt{1+\Gamma^2}$$

so the eigenvalues will be $\lambda_0 = \sqrt{1+\Gamma^2}$, $\lambda_1 = -\sqrt{1+\Gamma^2}$ and it's matrix

$$\mathbb{D} = \begin{pmatrix} \sqrt{1+\Gamma^2} & 0 \\ 0 & -\sqrt{1+\Gamma^2} \end{pmatrix}$$

Now calculate the eigenvectors,

λ_0:

$$\begin{pmatrix} 1-\sqrt{1+\Gamma^2} & \Gamma \\ \Gamma & -(1+\sqrt{1+\Gamma^2}) \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = 0$$

$$\begin{aligned} (1-\sqrt{1+\Gamma^2})a + \Gamma b &= 0 \\ \Gamma a - (1+\sqrt{1+\Gamma^2})b &= 0 \end{aligned} \longrightarrow \vec{v}_0 = C_0\begin{pmatrix} 1 \\ -\dfrac{1-\sqrt{1+\Gamma^2}}{\Gamma} \end{pmatrix}$$

Normalizing

$$C_0 = \frac{1}{\sqrt{1+\left(\frac{1-\sqrt{1+\Gamma^2}}{\Gamma}\right)^2}} = \cos(\theta) \quad \& \quad \operatorname{sen}\theta = \frac{\frac{1-\sqrt{1+\Gamma^2}}{\Gamma}}{\sqrt{1+\left(\frac{1-\sqrt{1+\Gamma^2}}{\Gamma}\right)^2}}$$

then

$$\vec{v}_0 = \begin{pmatrix} \cos(\theta) \\ -\operatorname{sen}(\theta) \end{pmatrix}$$

λ_1:

$$\begin{pmatrix} 1+\sqrt{1+\Gamma^2} & \Gamma \\ \Gamma & -1+\sqrt{1+\Gamma^2} \end{pmatrix}\begin{pmatrix} c \\ d \end{pmatrix} = 0 \quad \rightarrow \quad \begin{matrix} (1+\sqrt{1+\Gamma^2})\,c + \Gamma d = 0 \\ \Gamma c + (-1+\sqrt{1+\Gamma^2})\,d = 0 \end{matrix}$$

Solving

$$\vec{v}_1 = C_1 \begin{pmatrix} \dfrac{1-\sqrt{1+\Gamma^2}}{\Gamma} \\ 1 \end{pmatrix}$$

Normalazing

$$C_1 = \frac{1}{\sqrt{1+\left(\dfrac{1-\sqrt{1+\Gamma^2}}{\Gamma}\right)^2}} = \cos(\theta) \quad \& \quad \operatorname{sen}\theta = \frac{\dfrac{1-\sqrt{1+\Gamma^2}}{\Gamma}}{\sqrt{1+\left(\dfrac{1-\sqrt{1+\Gamma^2}}{\Gamma}\right)^2}}$$

Then $\vec{v}_1 = \begin{pmatrix} \operatorname{sen}(\theta) \\ \cos(\theta) \end{pmatrix}$ and the matrix

$$\mathbb{R} = \begin{pmatrix} \cos\theta & \operatorname{sen}\theta \\ -\operatorname{sen}\theta & \cos\theta \end{pmatrix}, \quad \mathbb{R}^+ = \begin{pmatrix} \cos\theta & -\operatorname{sen}\theta \\ \operatorname{sen}\theta & \cos\theta \end{pmatrix}$$

Therefore the time evolution operator will be

$$U = \mathbb{R}^+ e^{-\frac{i}{\hbar}\mathbb{D}t}\,\mathbb{R} \qquad \text{with } \phi = \sqrt{1+\Gamma^2}\; t/\hbar$$

$$= \begin{pmatrix} \cos\theta & -\operatorname{sen}\theta \\ \operatorname{sen}\theta & \cos\theta \end{pmatrix}\begin{pmatrix} e^{-i\phi} & 1 \\ 1 & e^{i\phi} \end{pmatrix}\begin{pmatrix} \cos\theta & \operatorname{sen}\theta \\ -\operatorname{sen}\theta & \cos\theta \end{pmatrix}$$

$$= \begin{pmatrix} e^{-i\phi}\cos\theta - \operatorname{sen}\theta & \cos\theta - e^{i\phi}\operatorname{sen}\theta \\ e^{-i\phi}\operatorname{sen}\theta + \cos\theta & \operatorname{sen}\theta + e^{i\phi}\cos\theta \end{pmatrix}\begin{pmatrix} \cos\theta & \operatorname{sen}\theta \\ -\operatorname{sen}\theta & \cos\theta \end{pmatrix}$$

$$U = \begin{pmatrix} e^{-i\phi}\cos^2\theta + e^{i\phi}\operatorname{sen}^2\theta - \operatorname{sen}(2\theta) & 2\cos\phi\,\operatorname{sen}\theta\cos\theta + \cos^2\theta - \operatorname{sen}^2\theta \\ 2i\,\operatorname{sen}\phi\,\operatorname{sen}\theta\cos\theta + \cos^2 - \operatorname{sen}^2\theta & e^{-i\phi}\operatorname{sen}^2\theta + e^{i\phi}\cos^2\theta + \operatorname{sen}(2\theta) \end{pmatrix}$$

Then the state in any t time will be

$$|\psi(t)\rangle = e^{-\frac{i}{\hbar}\hat{H}t}|\psi(0)\rangle$$

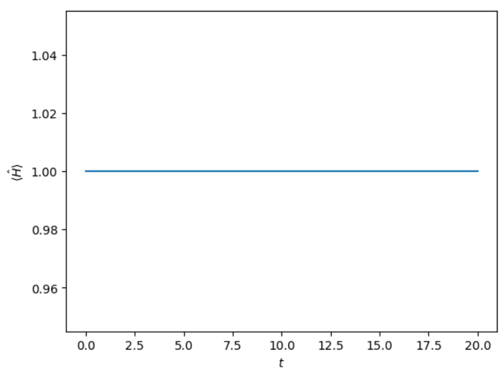
$$= \hat{R}^{+} e^{-\frac{i}{\hbar}\hat{D}t}\hat{R}\,|0\rangle$$

$$|\psi(t)\rangle = \left(e^{-\frac{i}{\hbar}\sqrt{1+\Gamma^2}\,t}\cos^2\theta + e^{\frac{i}{\hbar}\sqrt{1+\Gamma^2}}\,sen^2\theta - sen(2\theta)\right)|0\rangle$$
$$+ \left(2i\, sen\left(\frac{\sqrt{1+\Gamma^2}\,t}{\hbar}\right) sen\theta\cos\theta + \cos^2\theta - sen^2\theta\right)|1\rangle$$

where we can see clearly that $T = \frac{\pi\hbar}{\sqrt{1+\Gamma^2}}$

And of course $\langle\hat{H}\rangle = 1$

then the plot will be

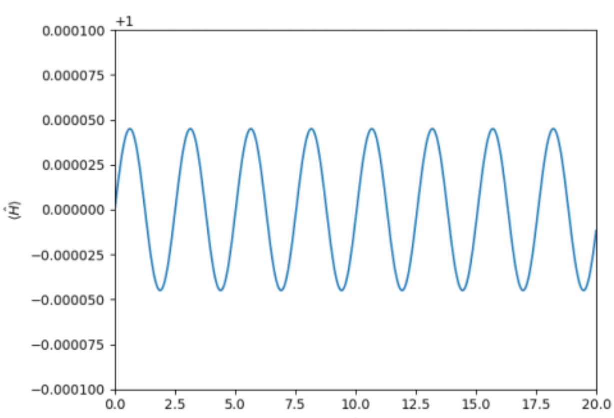


constant in time

b) Now using the Suzuki-Trotter approximant

$$\hat{U}(t+\Delta t; t) \approx e^{-i\Delta t\hat{\sigma}_z}\, e^{-i\Delta t\Gamma\hat{\sigma}_x}$$

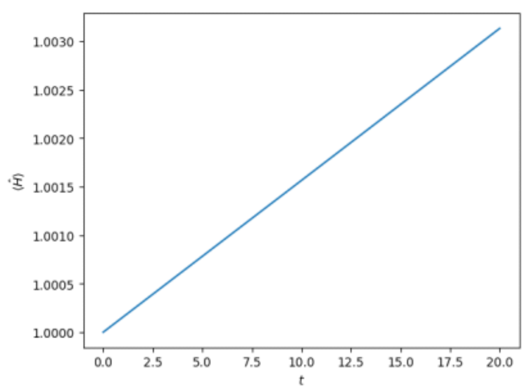
Give us



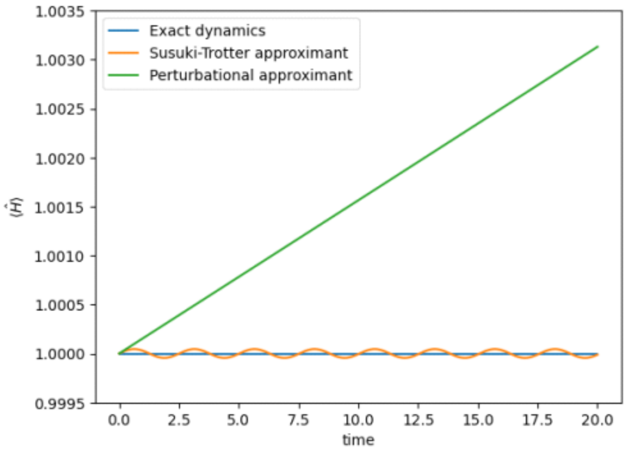
c) And the perturbational approximant

$$\hat{U}(t+\Delta t; t) \approx \hat{I} - i\Delta t\,\hat{H} = \hat{I} - i\Delta t(\hat{\sigma}_z + \Gamma\hat{\sigma}_x)$$

Give us



Then comparing the three results we have



Then, in this figure we can see the three solutions to the previous problem, of this we can conclude that both solutions Susuki-trotter and perturbational approximant are good approximations to calculate the energy of the system since the solutions only differ in 10^(-3) u and 10^(-4) u for perturbational and susuki-trotter respectively at least in the first 20 seconds.
However we can see clearly that the perturbational approximant doesn't converge since the solutions is proportional to the time, so while the time increase also will do the energy and that conclusion is physically impossible since that for a infinite time we will have infinite energy. Now this problem is due to the fact that the time-evolution operator in this case is not hermitian, therefore a non hermitian operator give us solutions or information that we cannot interpret, like imaginary energies, infinite energies etc. Then the importance of having hermitian operators is in order to obtain results that we can analyze, interpret and predict, and in this case the perturbational approximant for large times doesn't satisfy it, unlike susuki-trotter, that despite the exact solution doesn't oscillate, this give us an idea of how can be the real solution with quite precision.

3) In this case we have the system

$$K(\vec{p}) = \frac{1}{2}(\vec{p}_1^{\,2} + \vec{p}_2^{\,2}) \quad \text{and} \quad V(\vec{q}) = \frac{1}{2} q_1^2 q_2^2$$

with the initial conditions $q_1 = 2$, $q_2 = 1$ and $p_1 = p_2 = 0$ and $\Delta t = 0.0001$
Then remember the approximations seen

Trotter approximant

$$\begin{pmatrix} \vec{p}(t) \\ \vec{q}(t) \end{pmatrix} = e^{\Delta t \mathcal{H}} \begin{pmatrix} p(0) \\ q(0) \end{pmatrix} \quad \Rightarrow \quad e^{\Delta t \mathcal{H}} \approx e^{\Delta t \mathcal{K}} e^{\Delta t \mathcal{V}}$$

where

$$\mathcal{K} = \begin{pmatrix} 0 & 0 \\ \hat{K}\cdot & 0 \end{pmatrix} \qquad \mathcal{V} = \begin{pmatrix} 0 & -\hat{V}\cdot \\ 0 & 0 \end{pmatrix}$$

and as $\mathcal{K}^2 = \mathcal{V}^2 = 0$, then $e^{\Delta t \mathcal{K}} = I + \Delta t \mathcal{K}$ &
$e^{\Delta \mathcal{V}} = I + \Delta t \mathcal{K}$, therefore

$$\begin{pmatrix} \vec{p}(t) \\ \vec{q}(t) \end{pmatrix} = (I + \Delta t \mathcal{K})(I + \Delta t \mathcal{V}) \begin{pmatrix} \vec{p}^{(0)} \\ \vec{q}^{(0)} \end{pmatrix}$$

$$= \begin{pmatrix} 1 & 0 \\ \hat{K}\cdot & 1 \end{pmatrix} \begin{pmatrix} 1 & -\Delta t \hat{V}\cdot \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \vec{p}^{(0)} \\ \vec{q}^{(0)} \end{pmatrix}$$

$$= \begin{pmatrix} 1 & 0 \\ \hat{K}\cdot & 1 \end{pmatrix} \begin{pmatrix} \vec{p}^{(0)} - \Delta t \frac{d}{d\vec{q}} V(\vec{q}^{(0)}) \\ \vec{q}^{(0)} \end{pmatrix}.$$

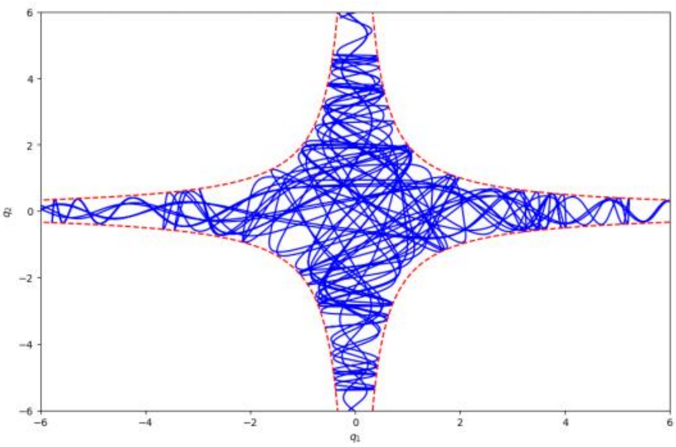
$$\begin{pmatrix} \vec{p}^{(1)} \\ \vec{q}^{(1)} \end{pmatrix} = \begin{pmatrix} \vec{p}^{(0)} - \Delta t \frac{d}{d\vec{q}} V(\vec{q}^{(0)}) \\ \vec{q}^{(0)} + \Delta t \frac{d}{d\vec{p}} K(\vec{p}^{(1)}) \end{pmatrix} \quad \text{with} \quad \vec{p}^{(1)} = \vec{p}^{(0)} - \Delta t \frac{d}{d\vec{q}} V(\vec{q}^{(0)})$$

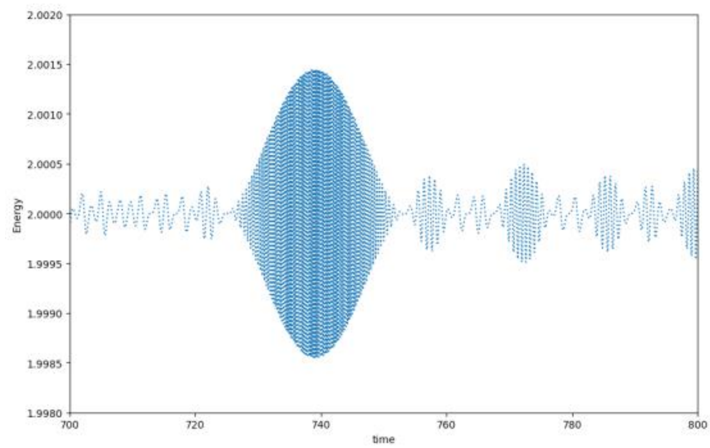
Then the iteration for each particle will be

$$p_1^{(n)} = p_1^{(n-1)} - \Delta t \frac{d}{dq_1} V(\vec{q}^{(n-1)}) \;,\quad p_2^{(n)} = p_2^{(n-1)} - \Delta t \frac{d}{dq_2} V(\vec{q}^{(n-1)})$$

$$q_1^{(n)} = q_1^{(n-1)} + \Delta t \frac{d}{dp_1} K(\vec{p}^{(n)}) \;,\quad q_2^{(n)} = q_2^{(n-1)} + \Delta t \frac{d}{dp_2} K(\vec{p}^{(n)})$$

Therefore using this approximation, we obtain the following pictures





And we can see that of course the phase diagram follow the same form that the paper analyzed, confined in a specific region given by $|q_1 q_2| = 2$ in a time $700 \leq t \leq 900$. And also the energy in function of time that oscillate around to $E=2$ which is the initial and theoretical value for whole dynamics, but because at the end the trotter approximant is an approximation the value is not exactly the same but with error less than 0.001 approximately.

Perturbational approximant

Here the approximation directly in the exponential of the hamiltonian

$$\begin{pmatrix} \vec{p}^{(1)} \\ \vec{q}^{(1)} \end{pmatrix} = e^{\Delta \mathcal{H}} \begin{pmatrix} \vec{p}^{(0)} \\ \vec{q}^{(0)} \end{pmatrix} \approx (I + \Delta t \mathcal{H}) \begin{pmatrix} \vec{p}^{(0)} \\ \vec{q}^{(0)} \end{pmatrix} \ldots$$

$$\ldots = \begin{pmatrix} 1 & -\Delta t \hat{V} \cdot \\ \Delta t \hat{K} \cdot & 1 \end{pmatrix} \begin{pmatrix} \vec{p}^{(0)} \\ \vec{q}^{(0)} \end{pmatrix} = \begin{pmatrix} \vec{p}^{(0)} - \Delta t \frac{d}{d\vec{q}} V(\vec{q}^{(0)}) \\ \vec{q}^{(0)} - \Delta t \frac{d}{d\vec{p}} K(\vec{p}^{(0)}) \end{pmatrix}$$

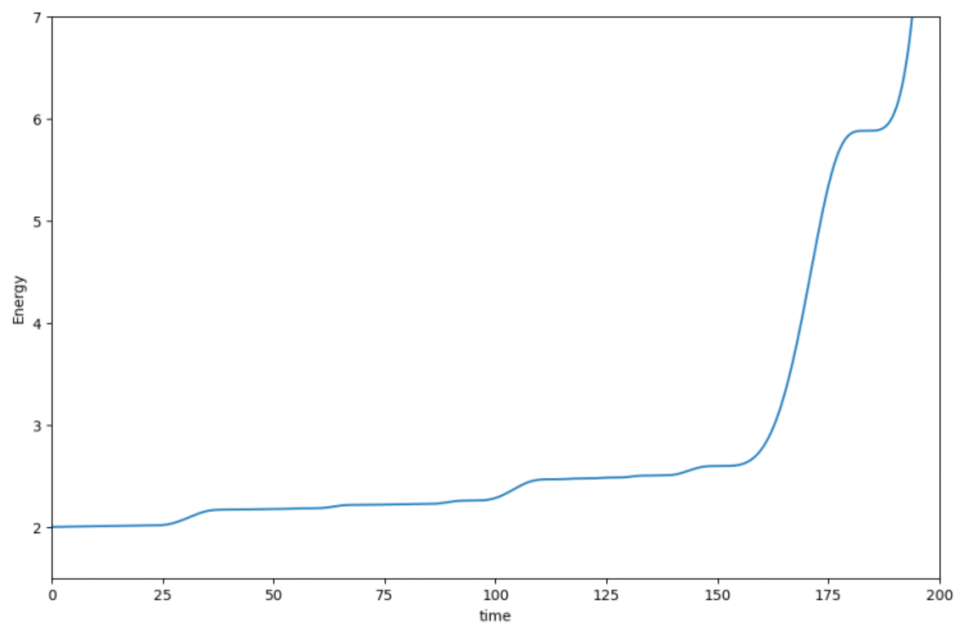
Then the iteration for each particle will be

$$p_1^{(n)} = p_1^{(n-1)} - \Delta t \frac{d}{dq_1} V(\vec{q}^{(n-1)}) \ , \quad p_2^{(n)} = p_2^{(n-1)} - \Delta t \frac{d}{dq_2} V(\vec{q}^{(n-1)})$$

$$q_1^{(n)} = q_1^{(n-1)} + \Delta t \frac{d}{dp_1} K(\vec{p}^{(n-1)}) \ , \quad q_2^{(n)} = q_2^{(n-1)} + \Delta t \frac{d}{dp_2} K(\vec{p}^{(n-1)})$$

Then the difference is only in the step for calculate $\vec{q}^{(i)}$ because now this is with $\vec{p}^{(i-1)}$ and not with $\vec{p}^{(i)}$

Therefore using this approximation, we obtain the following pictures



where we can see that the energy tends to infinity because again this is a non-unitary operator.