Phys Enph 479/879: Feynman's Quantum Path integral approach to modeling electron-phonon Scattering gives the numerical solution of time-dependent density matrix

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The Feynman's Quantum Path Integration connects the classical mechanics to quantum mechanics, which gives an intuitive description of qunatum mechanics. In this article, we solve one and two dimensional ground-state wavefunctions on isotropic harmonic oscillator computationally by using Feynman's Path Integral Monte Carlo approach with Metropolis and Lattice Quantum Mechanics algorithm. We have demonstrated analytical and numerical results of ground state wavefunction. The expectation values of x, x^2, x^3, x^4 and ground-state energy has been validate with the analytical solution. We find $\langle x\rangle = -0.0035$, $\langle x^2\rangle = 0.4981$, $\langle x^3\rangle = -0.0010$, $\langle x^4\rangle = 0.743$ and $E_0 = 0.494$. Then, we record the simulation time of 2D Feynman's Path Integration using Message Passing Interface (MPI) simulation and Numba (a source JIT compiler). We have tested ntasks = 1, 2, 4, 8, 16, and 23 for multiple nodes.

I. INTRODUCTION

The path integral approach has been applied in many different fields, for instance, polymer physics, quantum mechanics, quantum field theory, spring theory, and mainly Quantum chromodynamics (QCD). In this article, we are learning to solve one-dimensional, two-dimensional and three-dimensional ground-state wavefunctions using Feynman's Path Integral Monte Carlo approach with Metropolis algorithm (a computational method). We have compared our results with analytical solution for 1D and 2D ground-state wavefuntion.

In quantum mechanics, the Path Integral approach is varying the whole path from particle A to B, thus we can sum the probability of all the paths for a particle at position x_a at time t_a to position x_b at time t_b. The path integral allows to change coordinates easily under same quantum system. It is also easier to obtain a correct form of the Lagrangian of a theory than the Hamiltonian.

The article is organized as follows: in Sec. II we present the theoretical backgroud and derivation of 1D, 2D and 3D Feynman's Quantum Path Integration and computational implementation we use to solve the problem. We then demonstrate our results and effiency of the codes in MPI simulation with numba source in Sec. III. In the end, we conclude in Sec. IV.

In addition, we provide a appendix: Appendix A presents the derivation of numerical one-dimensional Feynman's Quantum Path Integral on Harmonic Oscillator.

II. THEORY AND COMPUTATIONAL IMPLEMENTATION

The general one-dimensional quantum wavefunction describe the propagation of a free particle in space-time representation is,

$$\psi(x_b,t_b) = \int dx_a G(x_b,t_b;x_a,t_a)\psi(x_a,t_a), \tag{1}$$

where, $G(x_b,t_b;x_a,t_a)$ is the propagator, or so called Green's function. The general Feynman's Quantum Path Integral can be written as,

$$G(b,a) = \sum_{\text{paths}} e^{iS[b,a]/\hbar}, \tag{2}$$

In Classical Mechanics, we have a path or classical trajectory from particle A to particle B in time-space reference. In Quantum Mechanics, we apply Hamilton's Principle of Least Action, thus we have a particle travels along the classical trajectory with other trajectory nearby, that we called extremum. Extremum means take the difference of action evaluate at a little away from the classical trajectory and action evaluate at the classical trajectory that is zero, thus, $\delta S[\overline{x}(t)] = S[\overline{x}(t) + \delta x(t)] - S[\overline{x}(t)] = 0$. It is shown in Figure 1.

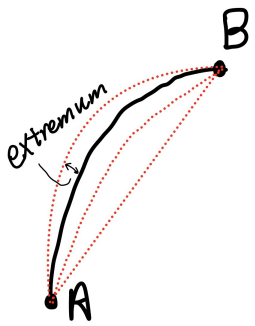

Figure 1. Path Integral qualitative representation for the connection between the initial state and final state. The black curve represents the classical trajectory, while the red dots are quantum trajectories.

Where all paths have to start at particle A and end at particle B. Hamilton's least-action principle is one of the most important principle in physics. One can derive Classical Mecahnics, Newton's Law, Einstein general relativity, optics etc. based on it.

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$S[x,\dot{x}]$ is the principle of least action (a function of space and time) and, where $[x,\dot{x}]$ is a functional. Hence, $S[x,\dot{x}]$ is functional of function of classical trajectory. It can be evaluate simply by taking integral of Lagrangian (L), with respect to time.

$$S[x,\dot{x}] = S[\overline{x}(t)] = \int dt\mathcal{L}[x(t),\dot{x}(t)], \tag{3}$$

where $\overline{x}(t)$ is a classical trajectory, $\mathcal{L}$ is Lagrangian, equals to $T[x,\dot{x}] - V[x]$. $T[x,\dot{x}]$ is kinetic energy of the particle. $V[x]$ is potential energy. Then, we need to apply Wick Rotation theorem to rotate the real time axis to imaginary time axis, $t \to -i\tau$. The Lagrangian becomes negative Hamiltonian,

$$L = \left[\frac{m}{2}\left(\frac{dx}{-id\tau}\right)^2 - V(x(t))\right] \tag{4}$$

$$= -\left[\frac{m}{2}\left(\frac{dx}{d\tau}\right)^2 + V(x(t))\right] = -\hat{H}. \tag{5}$$

Thus, we can rewrite the action as following equation,

$$S[x,\dot{x}] = \int_{t_i}^{t_f} dt\left[\frac{m}{2}\left(\frac{dx}{d\tau}\right)^2 + V(x(t))\right]. \tag{6}$$

In addition, the Path Integral (Green's function) becomes,

$$G(b,a) = \langle x_b,t_b|x_a,t_a\rangle = \int \mathcal{D}[x(t)]e^{-S[x]}. \tag{7}$$

A. Numeical one dimensional Feynman's Quantum Path Integration on the Harmonic oscillator

For 1D Harmonic Oscillator we have,

$$V(x) = \frac{1}{2}m\omega^2x^2. \tag{8}$$

We discretized the path into some infinitesimal links, then the action at a discretized path $\{x_i\}$ is,

$$S[x_i] = \frac{m}{2}\left[(x_{i+1}-x_i)^2 + (x_i - x_{i-1})^2\right] + \frac{1}{2}m\omega^2x_i^2. \tag{9}$$

For the details of the derivation please see Appendix A. The boundary condition is $x_0 = x_N = x$. Later, we will validate our numerical result with the anaylytical solution of 1D ground-state wavefunction with the Harmonic Oscillator, which is,

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\exp\left[-m\omega x^2\right]. \tag{10}$$

The energy of harmonic oscillator is,

$$E_n = \left(n+\frac{1}{2}\right)\hbar\omega. \tag{11}$$

We can also calculate the ground state energy through expectation of values,

$$E_0 = m\omega^2\sigma_x^2 = m\omega^2(\langle x^2\rangle - \langle x\rangle). \tag{12}$$

B. Numerical two and three dimensional Feynman's Quantum Path Integration on the isotropic Harmonic oscillator

The isotropic harmonic oscillator is,

$$V(x,y,z) = \frac{1}{2}m\omega^2(x^2+y^2+z^2). \tag{13}$$

Follow the similar derivation of 1D Path Integral (see Appendix A), we obtain two dimensional Path Integral on harmonic oscillator at a discretized path $\{x_i,y_i\}$ is,

$$\begin{aligned} S[x_i,y_i] = &\frac{m}{2}\left[(x_{i+1}-x_i)^2 + (x_i-x_{i-1})^2\right] \\ &+ \frac{m}{2}\left[(y_{i+1}-y_i)^2 + (y_i-y_{i-1})^2\right] \\ &+ \frac{1}{2}m\omega^2(x_i^2+y_i^2). \end{aligned} \tag{14}$$

The analytical solution of two dimensional ground-state wavefunction with harmonic oscillator is,

$$\psi_{n_x,n_y}(x,y) = \frac{\beta}{\sqrt{\pi(2)^{n_x+n_y}(n_x)!(n_y)!}}\exp\left(\beta^2(x^2+y^2)\right), \tag{15}$$

where $\beta = \sqrt{m\omega/\hbar}$. The three dimensional Path Integral on harmonic oscillator at a discretized path $\{x_i,y_i,z_i\}$ is,

$$S[r_i] = \frac{m}{2}\left[(r_{i+1}-r_i)^2 + (r_i-r_{i-1})^2\right] + \frac{1}{2}m\Omega^2r_i^2, \tag{16}$$

where $r_i = \sqrt{x_i^2+y_i^2+z_i^2}$.

C. The metropolis algorithm

The process is analogous to the Ising model, except the step of changing position is not limited to +1 and -1. A random number $\alpha = \epsilon\ [-\epsilon,\epsilon)$ is add to the time slice if the change is accepted. The following are the steps to update one path for a timestep:

1. Choose Number of steps in a path x, so j = Nsteps.
2. Create an index array with same length of the path and shuffle the order of it to update the path randomly.
3. Read the path by the order of the index, each time load the previous and next points.
4. Generate a random number $\alpha = \epsilon\ [-\epsilon,\epsilon)$ and add to the site x_j so that $x_j \to x_j + h * \alpha$, where h is the step size boundary (limit).
5. Calculate the change ΔS from old S and new S by using Eq (9), (14) or (16).
6. If $\Delta S < 0$ or a $\exp(-\Delta S)$ greater a random generate value [0,1), then update the change of site x_j and the "change rate" + 1.
7. Repeat step 2 to step 6 until all of the sites have been checked.

8. run step 1 to 7 with 100 timesteps in order to wait the system stabilized at some point.

In addition, all of the computational codes are written in Python with a version of 3.8, using Intel Core i7-7700HQ 2.80GHz CPU computer. In order to speed up the Path Integral Monte Carlo Python code, we have used a Python source, called numba. In addition, the 2D path integral Python code is written in parallel simulation, so one can simulation N number of paths in a same time.

III. RESULTS

A. One-dimensional Ground-state with Harmonic Oscillator via numerical solution of path Integrals

Now, we want to check our numerical results with analytical solutions. We set $dt = 0.3$ and simulate 5000 paths with 100 time slices. All the units are in term of dt, where $m = 1 * dt$ and $\omega = 1 * dt$. The initial path is generate randomly from NumPy package with a range of $\epsilon\ [-0.5, 0.5)$, using RANDOM.RAND() - 0.5. We obtain our thermalized path after runing the initial path for 100 timesteps by using metropolis algorithm Sec II C. Then we use Monte Carlo method to simulate 5000 paths using thermalized path. Figure 2 demonstrates the probability distribution of analytical and numerical results of ground-state wavefunction. The numerical result is plot in histogram with 500000 points and the analytical solution uses square of Eq. (10). Based on the presentation of Figure 2, our numerical result agrees with analytical result really well.

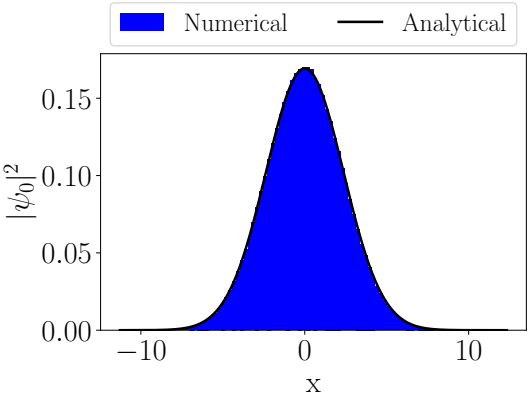

Figure 2. Comparison of numerical solution of 1D Feynman's Path Integral with analytical probability distribution of 1D ground-state wavefunction on Harmonic Oscillator, where numerical result is demonstrated in histogram with bins = 40, 5000 paths, 200 time slices and 100 timesteps; the black curve is analytical result obtain from square of Eq. (10)

Then, we calculate the expectation values by using the same data that plot Figure 2. The analytical expectation value of x, x^2 and x^3 for the stationary state is 0, 0.5 and 0. From our numerical result, we obtain,

$$\begin{aligned} \langle x \rangle &= -0.0035, \\ \langle x^2 \rangle &= 0.4981, \\ \langle x^3 \rangle &= -0.0010, \\ \langle x^4 \rangle &= 0.743. \end{aligned} \tag{17}$$

The results are very close to the analytical solution. We then calculate ground-state energy of harmonic oscillator with various Δt, which presents in Figure 3. Each Δt uses 1000 paths, 5000 time slices and 100 timesteps to simulate. Figure 3 shows, as Δt gets smaller, the more accurate result of ground-state energy we obtain. However, after many tests, the smaller Δt requires larger number of time slices and paths, so more cost of computing power, which is common in numerical implementation.

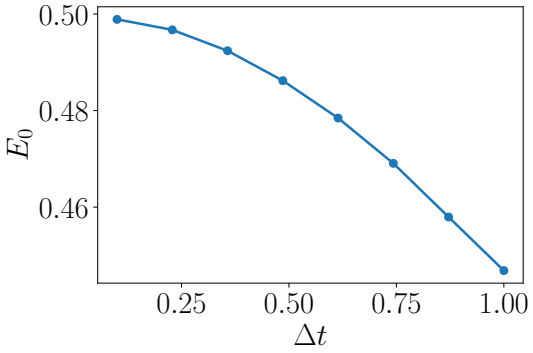

Figure 3. The ground-state energy calculation with various Δt, from 1D numerical Feynman's Quantum Path Integral Monte Carlo approach, 1000 paths, 5000 time slices and 100 timesteps.

B. two-dimensional Ground-state with Harmonic Oscillator via numerical solution of Feynman's Quantum Path Integration

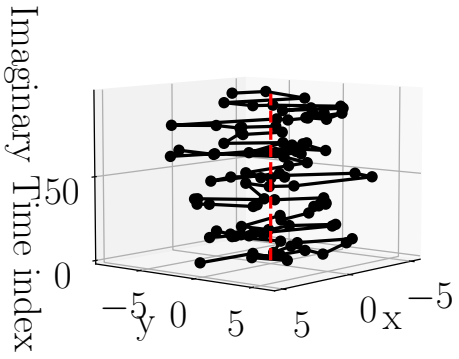

Figure 4. 3D plot of two dimensional Path over imaginary time for 100 time slices after 100 timesteps

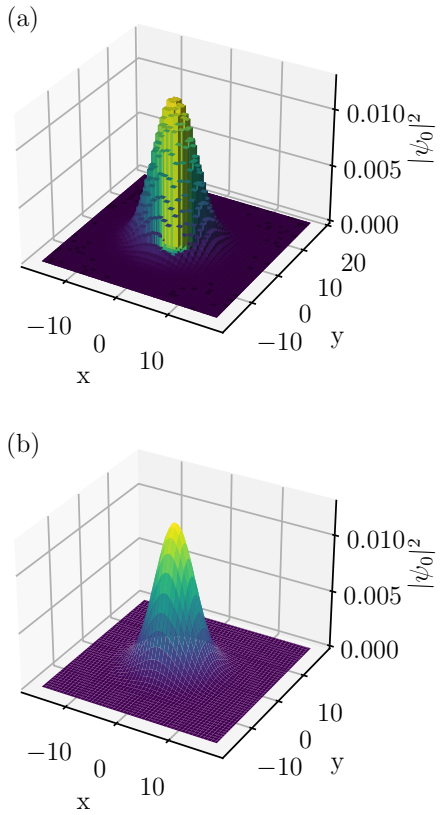

Figure 5. The three-dimensional plot of numerical and analytical probability distribution of 2D ground-state wavefunction on Harmonic Oscillator. a) numerical 2D Path for 10000 paths, 100 time slices and 100 timesteps and plot in histogram with bins = 40; b) analytical result from Eq. (15)

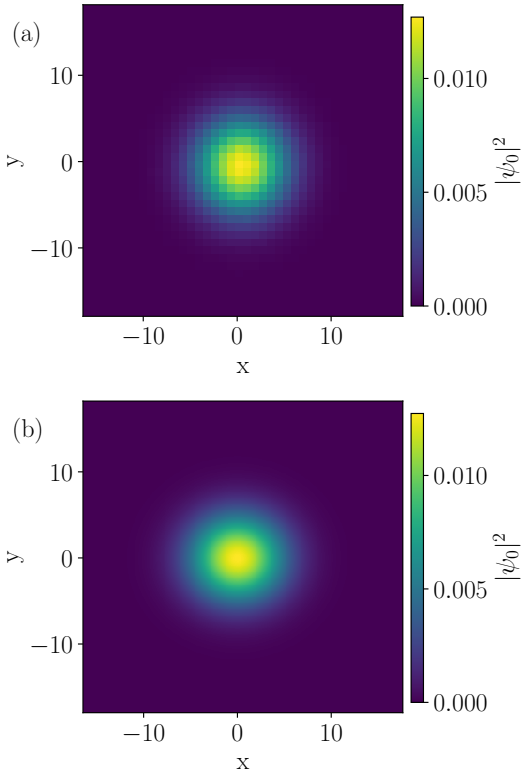

Figure 6. The two-dimensional plot of numerical and analytical probability distribution of 2D ground-state wavefunction on Harmonic Oscillator. a) numerical 2D Path for 10000 paths, 100 time slices and 100 timesteps and plot in histogram with bins = 40; b) analytical result from Eq. (15)

Processes	MPI numba Main (s)	MPI numba Linux
1	75.38	76.28
2	40.68	83.66
4	22.01	92.99
8	11.88	103.16
16	6.42	123.18
23	4.82	141.93

Table I. Parallelized simulation time of main code and Linux time (user + sys) of 2D Path Integral Monte Carlo with Numba for various number of processes with one single node. It takes 100 timesteps and 3680×3000 space grid points; the code is submitted to CAC Frontenac Cluster to simulate.

The two-dimensional numerical solution Feynman's Quantum Path Integration follows the similar computational implementation in 1D but using different formulation of action, Eq. (14). Figure 4 shows a single path in x, y, and imaginary time space with 100 time slices and 100 timesteps. After simulate 10000 paths we then obtain Figure 5. Figure 5 shows a 3D plot of probability distribution of analytical solution of 2D ground-state wavefunction and 2d Feynman Path Integral on Harmonic oscillator. Where Figure 6 presents the top view of 5. From the magnitude of 2D plots, which seem the numerical and analytical solution agrees with each other. However, the quality of the images of 2D plot of probability distribution changes after insert to Overleaf. To see a clear graph, please see the attachment.

Table I illustrates the simulation time of the main program and Linux time (user time + sys time) of parallel computation of 2D Feynman's Path Integral Monte Carlo approach on Harmonic Oscillator with numba source with various number of processors. The program simulates 3680 paths, 3000 time slices and 100 timesteps. As the number of processes increases, the simulation time of the main program decreases. However, it strange to see the Linux time increases as number of processes increases. We have also record the computational time with only MPI and only numba. They took 744.5 second for 23 cores and 68.62 second for single core with one single node. The simulation time with only MPI takes too loog for a run so we did not report it in this article.

The teaching account has maximum of 23 cores and 4 nodes, so we try to test the limit of the simulation time. Table II shows the simulation time of parallel computation of 2D Feynman's Path Integral Monte Carlo approach on Harmonic Oscillator with numba source with various number of processors (ntasks = 1, 2, 4, 8, 16, 23) and nodes (n = 1, 2, 3, 4). The fastest simulation is 23 cores with 4 nodes.

nodes	ntasks=23	ntasks=16	ntasks=8	ntasks=4	ntasks=2
1	4.82	6.42	11.88	22.01	40.68
2	2.99	3.71	6.27	11.48	20.85
3	2.39	2.87	4.7	7.94	14.38
4	1.96	2.43	3.66	6.28	10.8

Table II. Parallelized simulation time of main code of 2D Path Integral Monte Carlo with Numba for various number of nodes for different number of cores. It takes 100 timesteps and 3680 × 3000 space grid points; the code is submitted to CAC Frontenac Cluster to simulate.

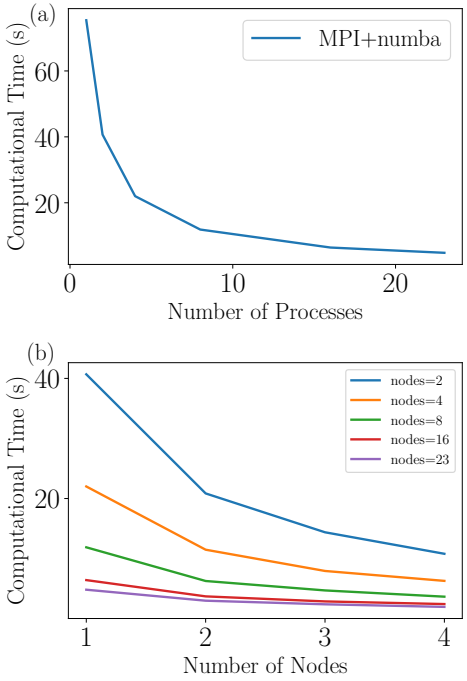

Figure 7. Computational simulation time of parallelized 2D Path Integral Monte Carlo with numba source Python code for a grid space points of 3680×3000 and 100 timesteps. (a) various number of cores (ntasks = 1, 2, 4, 8, 16, and 23) and one single nodes (data in Table I); (b) various number of nodes (n=1,2,3,4) for different number of cores (data in Tabel II

Figure 7 demonstrates the data of Table I and II. It is not surprise as number of processes or nodes increase, the speedup of the code become monotonically decreasing. One thing to be notice from Figure 7 (b), the computational time trends toward a different constant value, however, I expected as nodes large enough all the curves should overlap together.

IV. CONCLUSIONS

In this article, we have compared 1D and 2D Path Integral Monte Carlo approach with analytical solutions. We have also calculate the expectation value of x, x^2, x^3 and x^4, which are $\langle x\rangle = -0.0035$, $\langle x^2\rangle = 0.4981$, $\langle x^3\rangle = -0.0010$, $\langle x^4\rangle = 0.743$. The closest ground-state energy of harmonic oscillator from our calculation is $E_0 = 0.494$ from 1000 paths with 5000 time slices and 100 timesteps. We find the smaller Δt, the result is more accurate, however, it requires to simulate large number of time slices (links) and paths. The algorithm of the code is similar to Ising model, which cannot be vectorized. The fastest simulation time of 2D Path Integral code is given from 23 cores with 4 nodes and 3680×3000 grid space points, for 1.96 second. I may have find a way to obtain numerical first excitation plot from 3D Path Integral Monte Carlo approach. However, I am not sure whether the result is incorrect, I did not report here. For our Furthur investigation, we want to calculate numerical Green's function of 1D, 2D and 3D Path Integral and connect it with density matrix. Later, we can try to solve Path Integral with different Lagrangian model.

Appendix A: Derivation of one dimensional Path Integral on Harmonic Oscillator

To solve Feynman Path Integration numerically, we first want to apply lattice path integration algorithm to discretized Eq. (6) and split the paths into $N-1$ links. We discretized t axis:

$$t_j = t_i + j\Delta t, \qquad j = 0, 1, ..., N \tag{A1}$$

where Δt is the grid spacing,

$$\Delta t = \frac{t_f - t_i}{N}. \tag{A2}$$

Then a path is described by a set, $x = \{x(t_0), x(t_1), x(t_2), ..., x(t_N)\}$. Hence, we can write action as,

$$S[x] = \sum_{i=0}^{N-1}\left[\frac{m}{2\Delta t}(x_{i+1} - x_i)^2 + \Delta t V(x_i)\right]. \tag{A3}$$

We also want to evaluate the action at a discretized path $\{x_i\}$. We need to consider the $\{x_{i+1}\}$ and $\{x_{i-1}\}$, like Ising model, the neighour spins have effect on it. So the action for x_i becomes,

$$S[x_i] = \frac{m}{2}\left[(x_{i+1} - x_i)^2 + (x_i - x_{i-1})^2\right] + \frac{1}{2}m\omega^2 x_i^2. \tag{A4}$$

[1] K. Blum, "Density Matrix Theory and Applications" , *SSAOPP* **64** 3 (2012)

[2] R.H. Landau, M.J. Paez, C.C. Bordeianu, "A Survey of Computational Physics: Introductory Computational Sci-

ence", *PU press* 978–0–691–13137–5 (2007)
[3] M. Houtput and J. Tempere, "Beyond the Fröhlich Hamiltonian: Path-integral treatment of large polarons in anharmonic solids", *Phys. Rev. B* **103** 184306 (2021)
[4] T. Ichmoukhamedov and J. Tempere, "Feynman path-integral treatment of the Bose polaron beyond the Fröhlich model", *Phys. Rev. A* **100** 043605 (2019)
[5] G. Mazzi, "Numerical Treatment of the Liouville-von Neumann Equation for Quantum Spin Dynamics (2010)
[6] M. Riesh and C. Jirauschek, "Analyzing the positivity preservation of numerical methods for the Liouville-von Neumann equation, *J. Comput. Phys.* **390** 290-296 (2019)