Quantum Information Theory

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HT 1A: Statistical mechanics/Liouville equation

(Note: Results were supported by the mathematical software Python. See **quantum_info_theory.py)**

Let $\rho(t, q, p)$ be the density function of particles in the phase space (coordinates and momentum (q, p)). If the particles follow the trajectories given by the Hamiltonian function

$$\mathcal{H}(q, p) = p^2 + q^4$$

then, the dynamics of the density can be described by solving the Cauchy problem

$$\begin{cases} \frac{\partial \rho}{\partial t} = \{\mathcal{H}, \rho\} = 4q^3 \frac{\partial \rho}{\partial p} - 2p \frac{\partial \rho}{\partial q} \\ \rho(0, q, p) = \rho_0(q, p) \end{cases} \tag{1}$$

for some initial value ρ_0. Here we study the case where

$$\rho_0(q, p) = \frac{1}{2\pi} \exp\left(- \frac{q^2 + p^2}{2} \right)$$

We approximate the solution numerically by applying the finite differences method which computes the values

$$\rho^n_{i,j} \approx \rho(t_n, q_i, q_j)$$

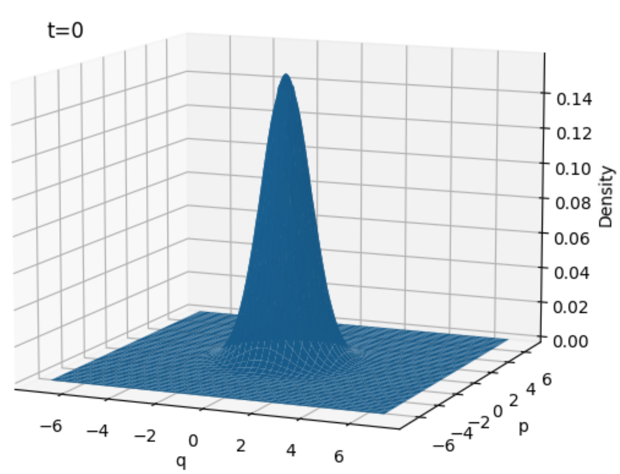
for a chosen partition of the phase space (q_i, p_j) and different times t_n. This reduces Liouville's partial differential equation to the algebraic equation

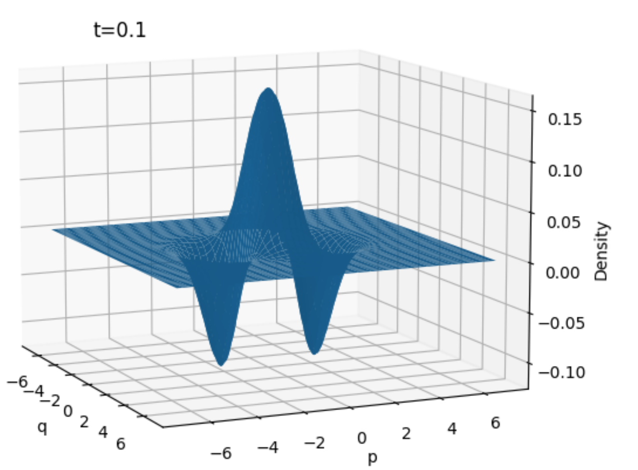
$$\frac{\rho^{n+1}_{i,j} - \rho^n_{i,j}}{\Delta t} = 4q_i^3 \frac{\rho^{n+1}_{i,j} - \rho^n_{i,j}}{\Delta p} - 2p_j \frac{\rho^{n+1}_{i,j} - \rho^n_{i,j}}{\Delta q}$$

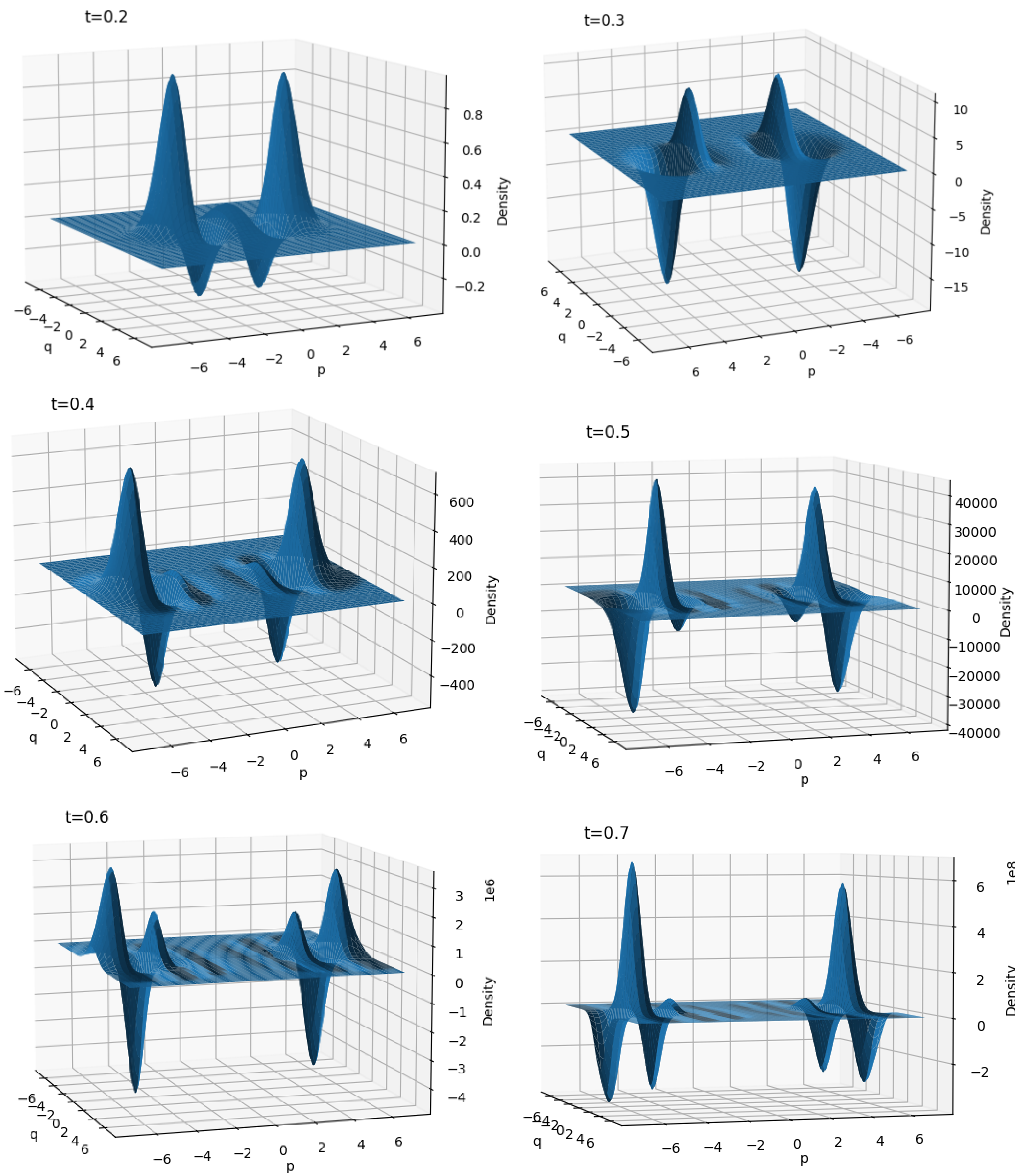
hence, given $\rho(t_n, q_i, p_j)$ we can approximate $\rho(t_{n+1}, q_i, p_j)$ by computing

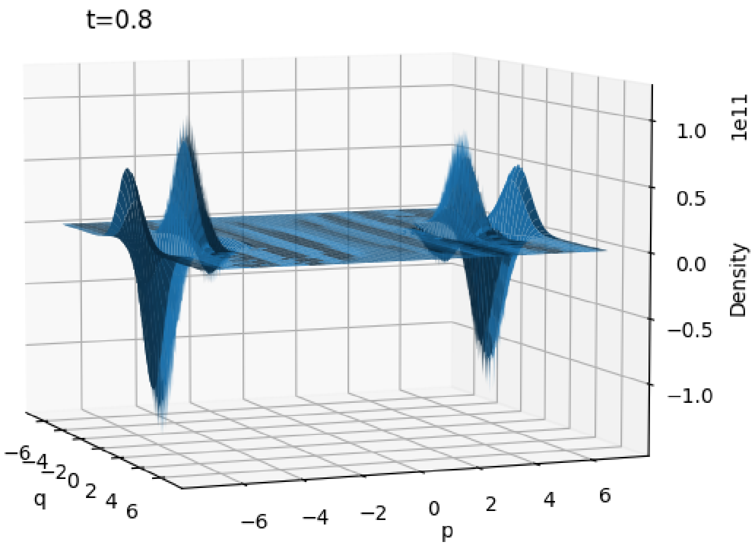
$$\rho^{n+1}_{i,j} = \Delta t \left(4q_i^3 \frac{\rho^{n+1}_{i,j} - \rho^n_{i,j}}{\Delta p} - 2p_j \frac{\rho^{n+1}_{i,j} - \rho^n_{i,j}}{\Delta q} \right) + \rho^n_{i,j}$$

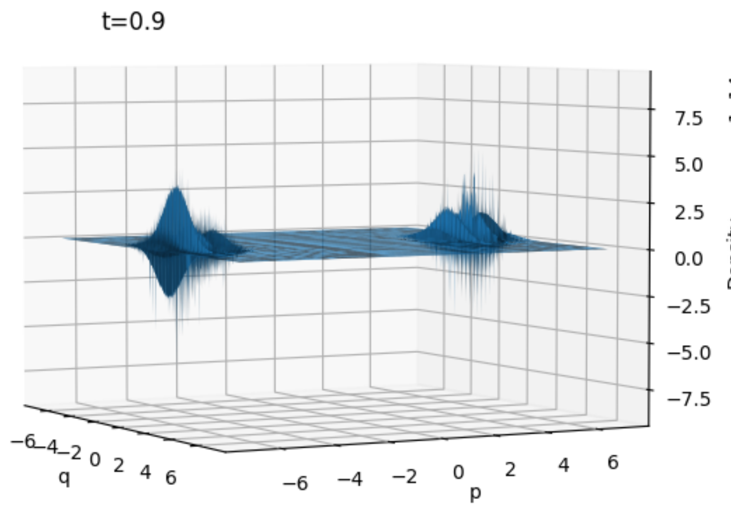
We try the simulation with the parameters $\Delta q = \Delta p = 0.01$ and $\Delta t = 0.1$. There's some dimensional analysis needed for expressing t in seconds, for instance using the LMT system, but here we simply show the evolution in time of the solution of (1).

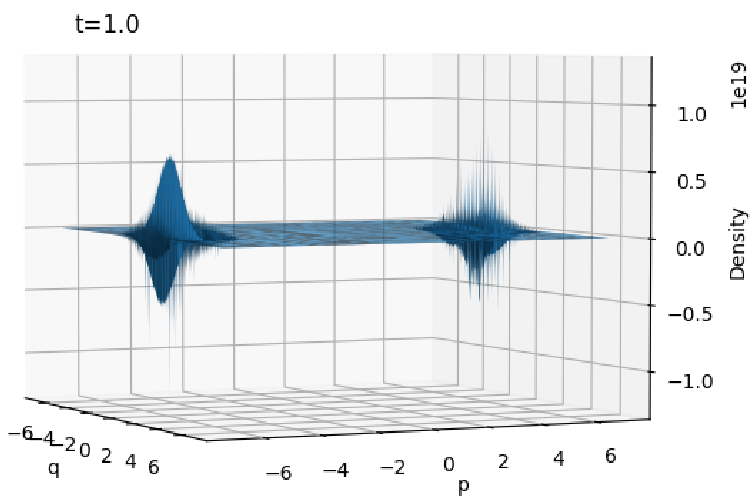





t=0.2
t=0.3
t=0.4
t=0.5
t=0.6
t=0.7
q
p
Density
1e6
1e8







The approximated density soon explodes to $\pm\infty$ so we ask ourselves if this is due to the unstableness of the finite differences method (due to the accumulating derivative and rounding errors) or if the solution actually behaves in that manner. To be sure, further study in partial differential equations should be done.