Quantum Simulations

The Center for the Hopelessly Naïve (CHN)

Simulation Model : Case 1

Dynamics

$$\hbar \frac{\partial x}{\partial t} = -iHx$$

$$y = \begin{bmatrix} 1 & 0 \end{bmatrix} x$$

*For this simulation, the Planck's constant was set to 1.

Eigenvalues of H:

$$\sigma(H) = \{1+\alpha, 1-\alpha\}$$

Hamiltonian:

$$H = \sigma_0 + \alpha\sigma_2 = \begin{bmatrix} 1 & -i\alpha \\ i\alpha & 1 \end{bmatrix}$$

Initial Conditions

$$X \equiv \mathbf{C}^2 \ \& \ X = \mathrm{span}\{\phi_1, \phi_2\}$$

Orthonormal basis vectors (eigen vectors of H):

$$\phi_1 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ i \end{bmatrix} \quad \phi_2 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -i \end{bmatrix} \quad (\phi_1, \phi_2) = 0$$

Initial condition:

$$x(0) = \cos(\theta)\ \phi_1 + \sin(\theta)\ \phi_2$$

Solver

Dormand & Prince (DOPRI5(4)) in solve_ivp(…..) from SciPy.

method : *string or OdeSolver, optional*

Integration method to use:

- 'RK45' (default): Explicit Runge-Kutta method of order 5(4) [1]. The error is controlled assuming accuracy of the fourth-order method, but steps are taken using the fifth-order accurate formula (local extrapolation is done). A quartic interpolation polynomial is used for the dense output [2]. Can be applied in the complex domain.

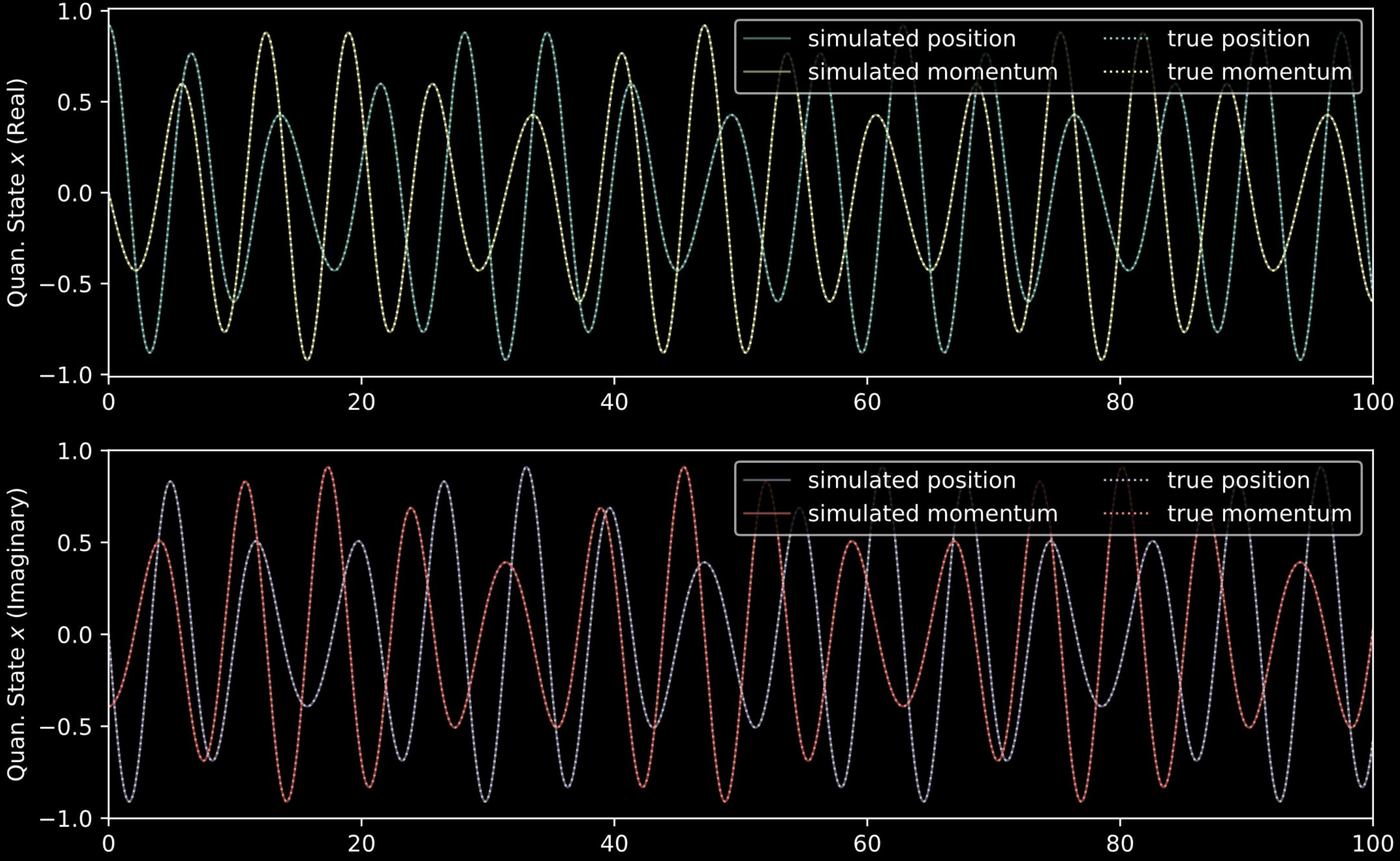
Verification

Verify the simulation output against the true solution:

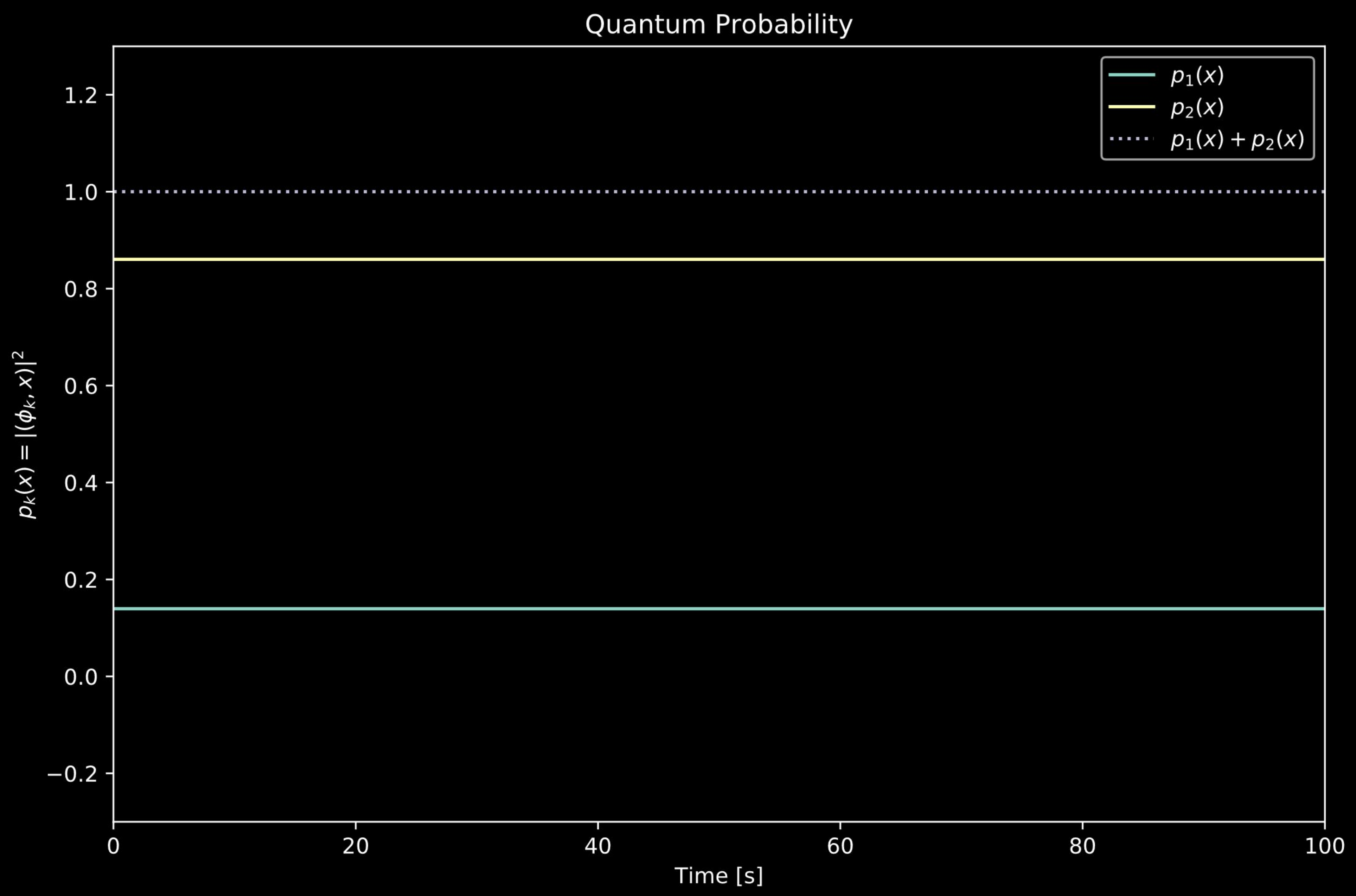
$$x(t) = e^{-i(1+\alpha)t}(\phi_1, x_0)\phi_1 + e^{-i(1-\alpha)t}(\phi_2, x_0)\phi_2$$

Also, verify the probabilities:

$$p_s(x) \equiv \|P_s x\|^2 = \sum_{k=1}^{2} |(\phi_k, x)|^2$$



Quan. State x (Real)
simulated position
simulated momentum
true position
true momentum
1.0
0.5
0.0
−0.5
−1.0
0
20
40
60
80
100
Quan. State x (Imaginary)
simulated position
simulated momentum
true position
true momentum
1.0
0.5
0.0
−0.5
−1.0
0
20
40
60
80
100


Quantum Probability
$p_1(x)$
$p_2(x)$
$p_1(x) + p_2(x)$
1.2
1.0
0.8
0.6
0.4
0.2
0.0
−0.2
$p_k(x) = |(\phi_k, x)|^2$
0
20
40
60
80
100
Time [s]

Simulation Model : Case 2

Dynamics

$$\hbar \frac{\partial x}{\partial t} = -iHx$$

$$y = \begin{bmatrix} 1 & 0 \end{bmatrix} x$$

Pauli Matrices:

$$\sigma_2 = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \quad \sigma_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \quad \sigma_3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \quad \sigma_0 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$\boxed{H = \sigma_0 + 0.01\,\sigma_1 + 0.1\,\sigma_2 + 0.05\,\sigma_3 = \begin{bmatrix} 1.05 & 0.01 - i\,0.1 \\ 0.01 + i\,0.1 & 0.95 \end{bmatrix}}$$

Initial Conditions

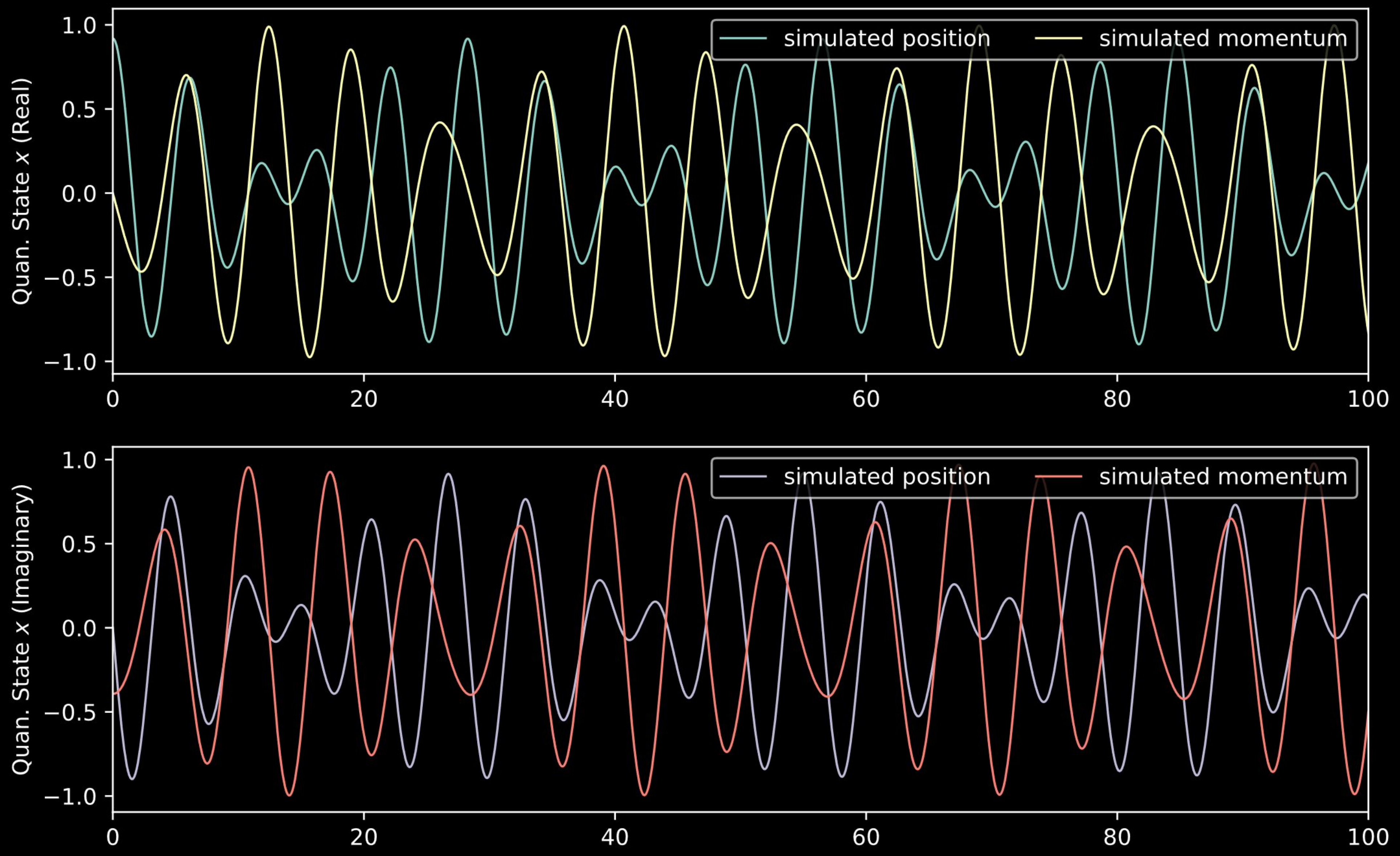
$$\mathrm{X} \equiv \mathbf{C}^2 \;\&\; \mathrm{X} = \mathrm{span}\{\phi_1, \phi_2\}$$

Orthonormal basis vectors:

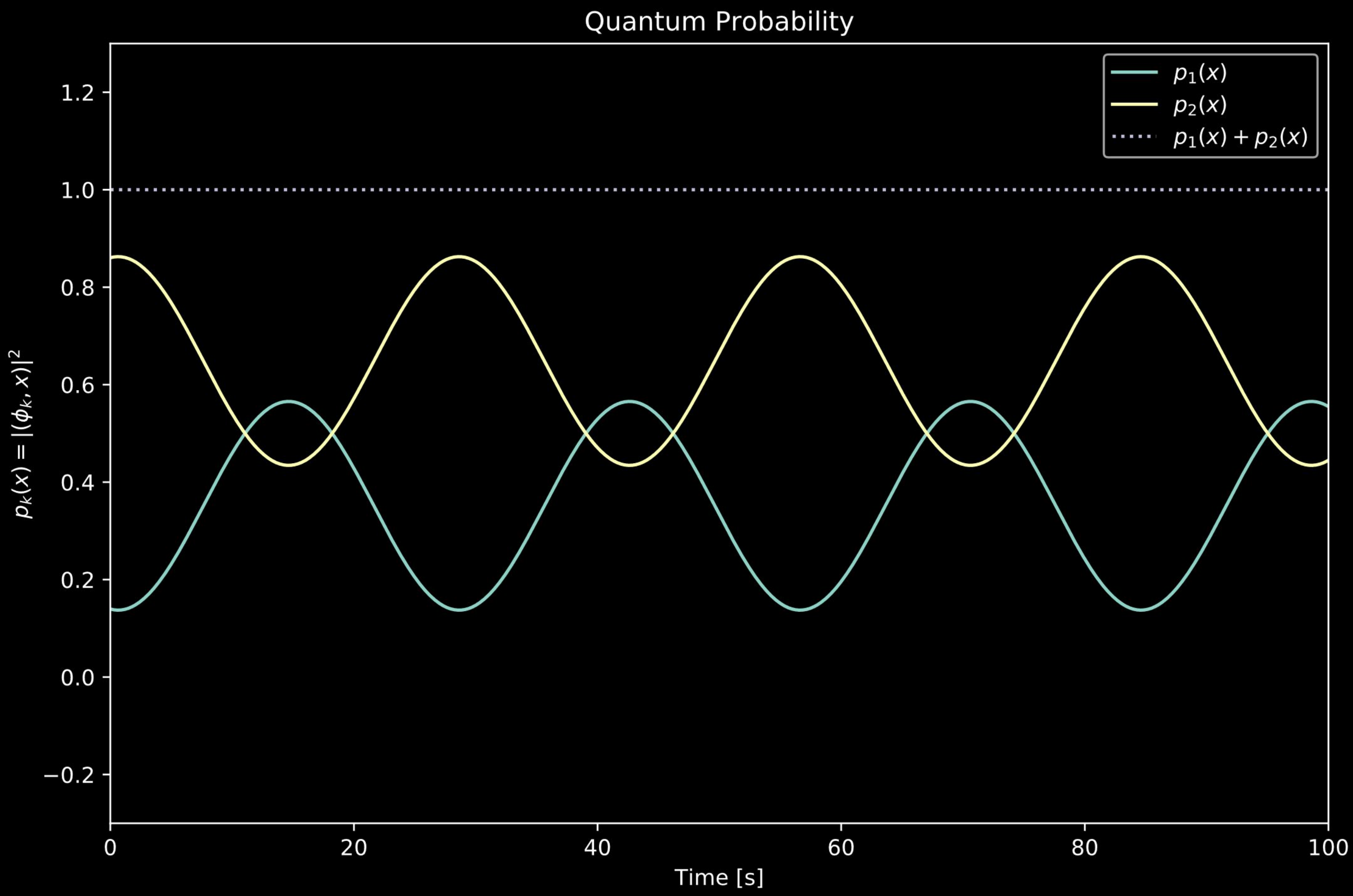
$$\phi_1 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ i \end{bmatrix} \quad \phi_2 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -i \end{bmatrix} \qquad (\phi_1, \phi_2) = 0$$

Initial condition:

$$\boxed{x(0) = \cos(10)\ \phi_1 + \sin(10)\ \phi_2}$$

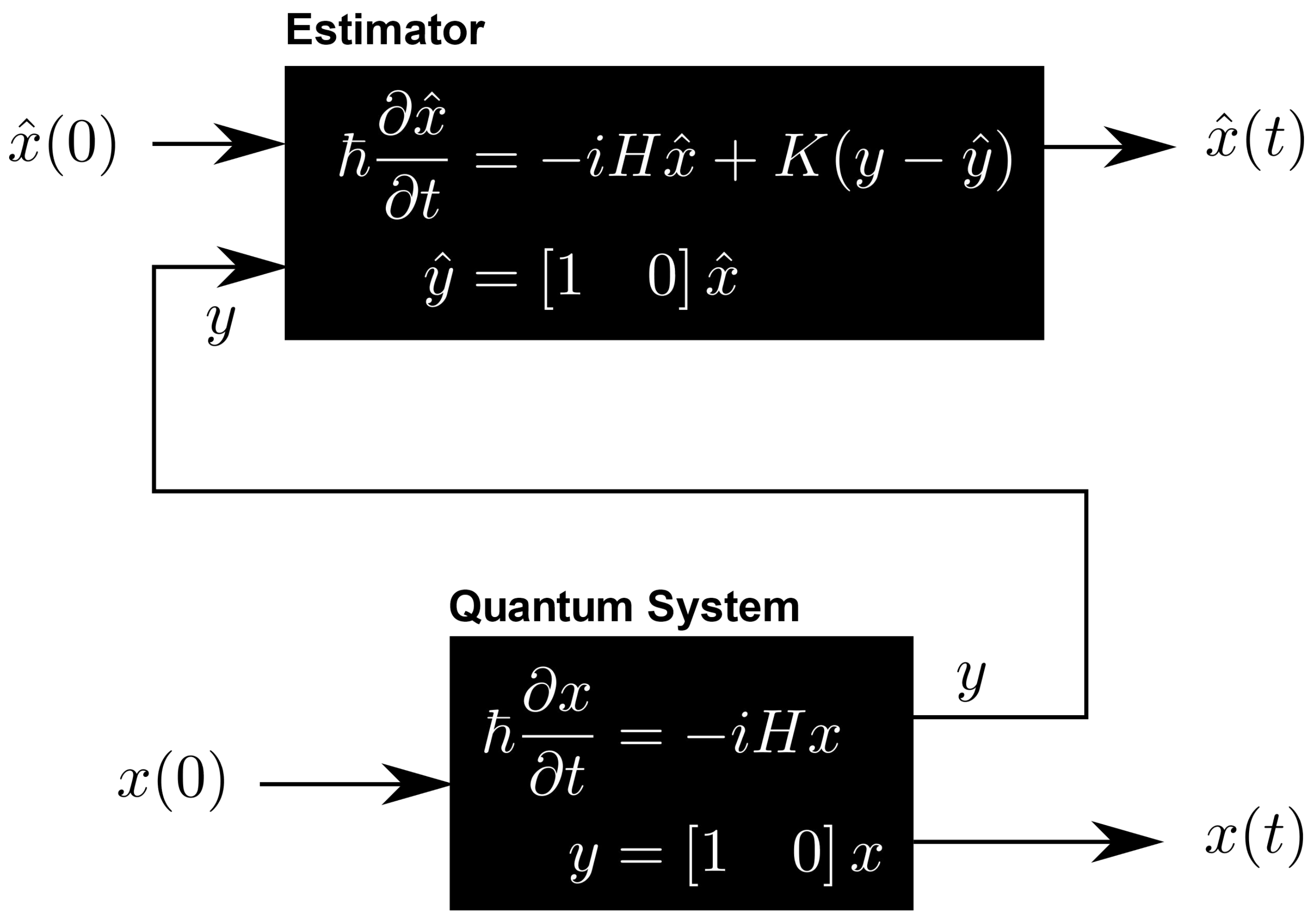


simulated position
simulated momentum
Quan. State x (Real)
1.0
0.5
0.0
−0.5
−1.0
0
20
40
60
80
100
simulated position
simulated momentum
Quan. State x (Imaginary)
1.0
0.5
0.0
−0.5
−1.0
0
20
40
60
80
100


Quantum Probability
$p_1(x)$
$p_2(x)$
$p_1(x) + p_2(x)$
1.2
1.0
0.8
0.6
0.4
0.2
0.0
−0.2
$p_k(x) = |(\phi_k, x)|^2$
0
20
40
60
80
100
Time [s]

Simulation Model : Case 3

Quantum Estimator



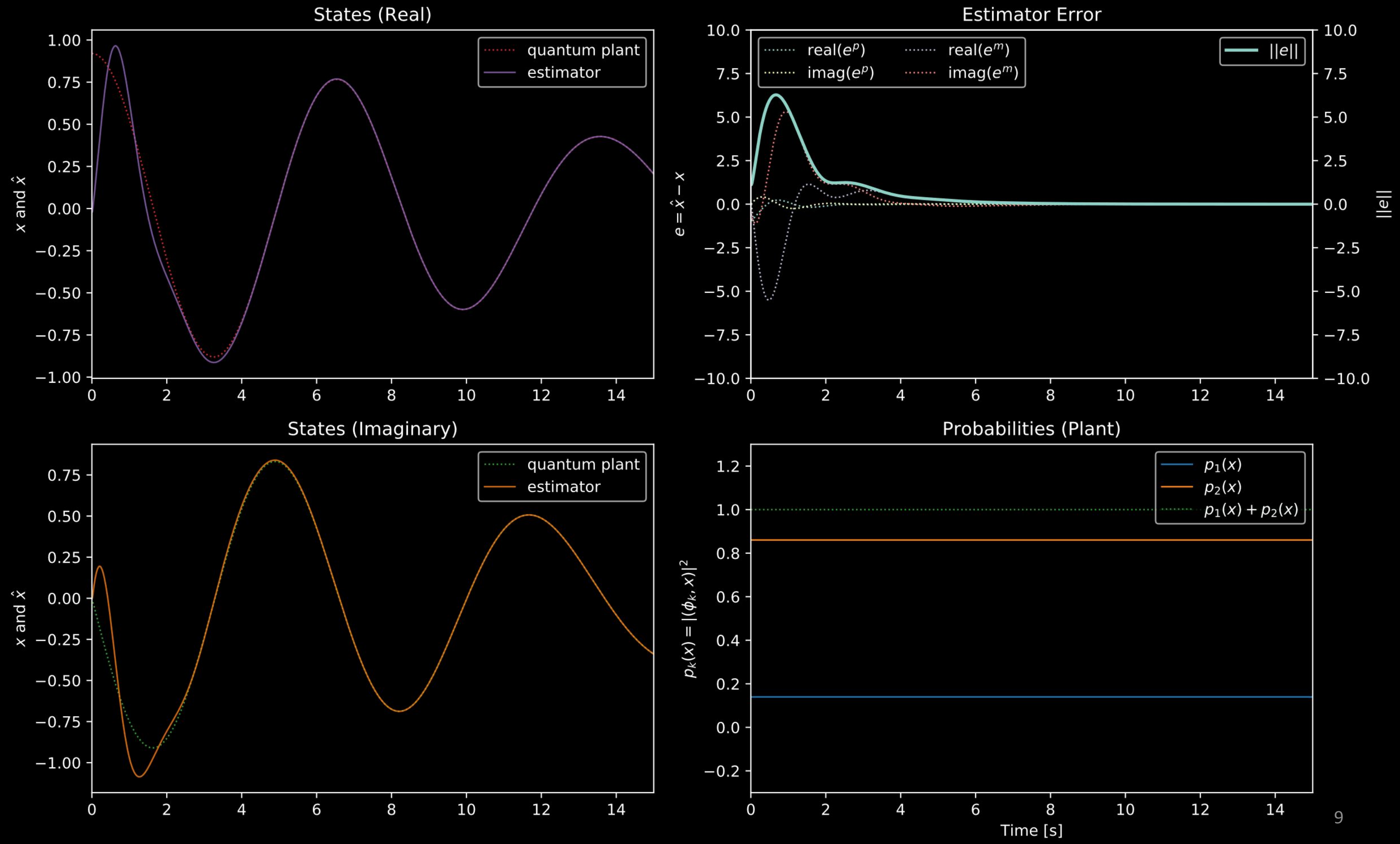
Estimator Gain

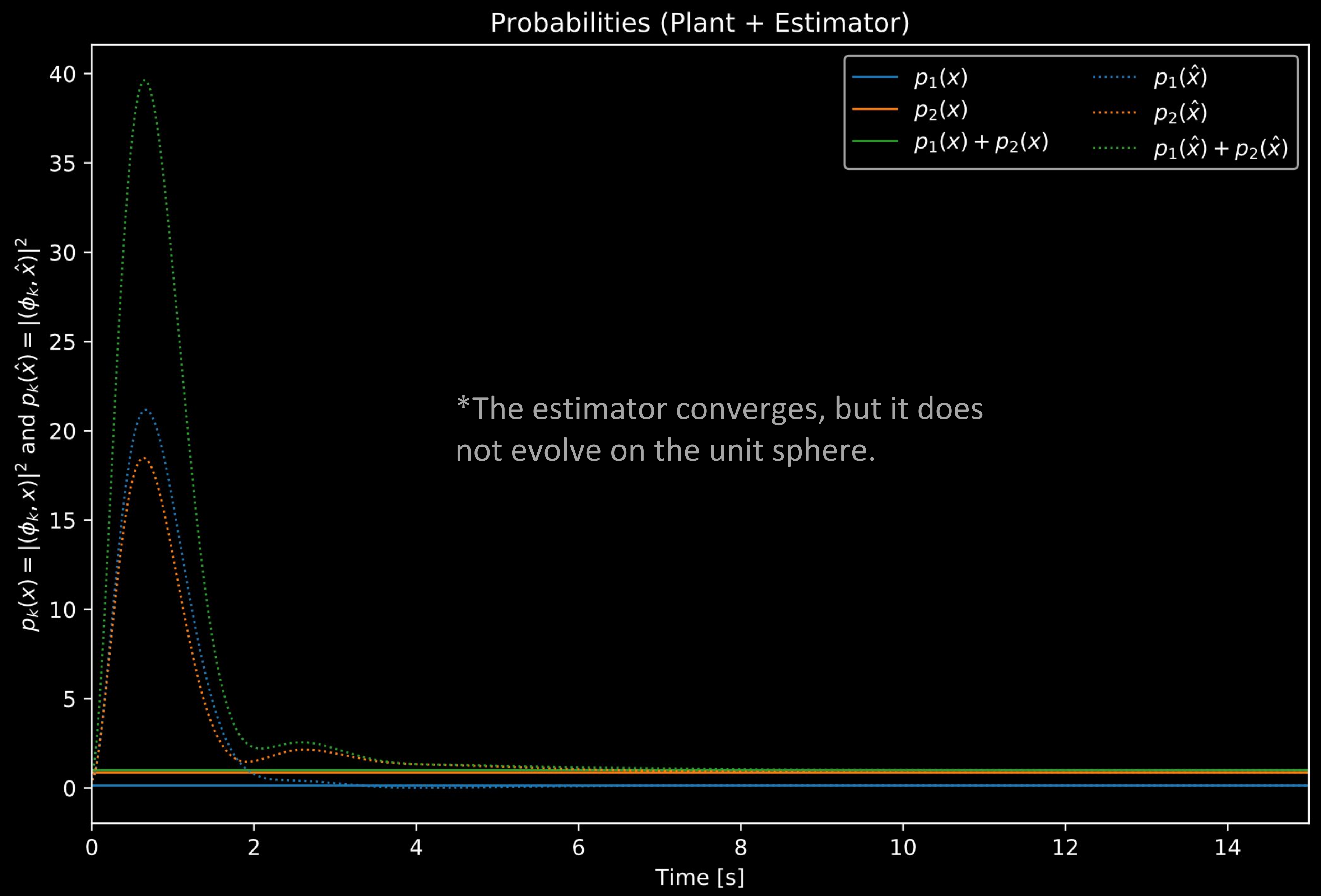
$$K = \begin{bmatrix} 2 + i2 \\ -\frac{2}{\alpha} + i\frac{\alpha^2 - 1}{\alpha} \end{bmatrix}$$

Estimator Error System

$$i\hbar \frac{\partial e}{\partial t} = (H - KC)e$$

$$K \ni \quad e \xrightarrow[t \to \infty]{} 0$$


States (Real)
quantum plant
estimator
x and $\hat{x}$
Estimator Error
real(e^p)
imag(e^p)
real(e^m)
imag(e^m)
$||e||$
$e = \hat{x} - x$
States (Imaginary)
quantum plant
estimator
x and $\hat{x}$
Probabilities (Plant)
$p_1(x)$
$p_2(x)$
$p_1(x) + p_2(x)$
$p_k(x) = |(\phi_k, x)|^2$
Time [s]



*The estimator converges, but it does not evolve on the unit sphere.