Exact solution for quantum-classical hybrid mode of a classical harmonic oscillator quadratically coupled to a degenerate two-level quantum system

The code in green should be uncommented (and the code in orange needs to be commented out) if one wants to study the general solution.

Settings

```
restart;
with(Physics):
```

Hamiltonian

$alias(H = H(q, p)):$

$alias\left(f_1 = f_1(q), f_2 = f_2(q), f_3 = f_3(q)\right):$

Wavefunction

$alias\left(\Upsilon_1 = \Upsilon_1(q, p, t), \Upsilon_2 = \Upsilon_2(q, p, t)\right):$

$\Upsilon := Vector\left(\left[\Upsilon_1, \Upsilon_2\right]\right):$

Pauli matrices

$alias\left(\sigma_1 = Library{:-}RewriteInMatrixForm(Psigma[1]), \sigma_2 = Library{:-}RewriteInMatrixForm(Psigma[2]), \sigma_3 = Library{:-}RewriteInMatrixForm(Psigma[3])\right):$

Quanutm-classical hybrid equation of motion for the Koopman wavefunction Υ

Hybrid equation of motion

$$HybridEq := -I\cdot\hbar\cdot\frac{\partial}{\partial t}\Upsilon - I\cdot\hbar\cdot\left(\frac{\partial}{\partial p}H\cdot\frac{\partial}{\partial q}\Upsilon - \frac{\partial}{\partial q}H\cdot\frac{\partial}{\partial p}\Upsilon - \left(\frac{\partial}{\partial q}f_1\cdot\sigma_1 + \frac{\partial}{\partial q}f_2\cdot\sigma_2 + \frac{\partial}{\partial q}f_3\cdot\sigma_3\right).\frac{\partial}{\partial p}\Upsilon\right) - \frac{1}{2}\cdot\left(q\cdot\frac{\partial}{\partial q}H\cdot\Upsilon + q\cdot\left(\frac{\partial}{\partial q}f_1\cdot\sigma_1 + \frac{\partial}{\partial q}f_2\cdot\sigma_2 + \frac{\partial}{\partial q}f_3\cdot\sigma_3\right).\Upsilon + p\cdot\frac{\partial}{\partial p}H\cdot\Upsilon\right) + H\cdot\Upsilon + \left(f_1\cdot\sigma_1 + f_2\cdot\sigma_2 + f_3\cdot\sigma_3\right).\Upsilon:$$

Hybrid density matrix expressed through the Koopman wave function

Define the matrix components of Hybrid density matrix

$$D_{1,1} := 2\cdot|\Upsilon_1|^2 + \Re\left(q\cdot\Upsilon_1\cdot\frac{\partial}{\partial q}conjugate(\Upsilon_1) + p\cdot\Upsilon_1\cdot\frac{\partial}{\partial p}conjugate(\Upsilon_1) + 2\cdot I\cdot\hbar\cdot\frac{\partial}{\partial q}\Upsilon_1\cdot\frac{\partial}{\partial p}conjugate(\Upsilon_1)\right):$$

$$D_{1,2} := 2\cdot\Upsilon_1\cdot conjugate(\Upsilon_2) + I\cdot\hbar\cdot\left(\frac{\partial}{\partial q}\Upsilon_1\cdot\frac{\partial}{\partial p}conjugate(\Upsilon_2) - \frac{\partial}{\partial q}conjugate(\Upsilon_2)\cdot\frac{\partial}{\partial p}\Upsilon_1\right) + \frac{\Upsilon_1}{2}\cdot\left(q\cdot\frac{\partial}{\partial q}conjugate(\Upsilon_2) + p\cdot\frac{\partial}{\partial p}conjugate(\Upsilon_2)\right) + \frac{conjugate(\Upsilon_2)}{2}\cdot\left(q\cdot\frac{\partial}{\partial q}\Upsilon_1 + p\cdot\frac{\partial}{\partial p}\Upsilon_1\right):$$

$$D_{2,2} := 2\cdot|\Upsilon_2|^2 + \Re\left(q\cdot\Upsilon_2\cdot\frac{\partial}{\partial q}conjugate(\Upsilon_2) + p\cdot\Upsilon_2\cdot\frac{\partial}{\partial p}conjugate(\Upsilon_2) + 2\cdot I\cdot\hbar\cdot\frac{\partial}{\partial q}\Upsilon_2\cdot\frac{\partial}{\partial p}conjugate(\Upsilon_2)\right):$$

Classical density

$$\rho_{classical} := D_{1,1} + D_{2,2}:$$

Density matrix for the quantum subsystem

$$\rho_{quant} := map\left(x\rightarrow Int(x, [q=-\infty..+\infty, p=-\infty..+\infty]), \begin{bmatrix} D_{1,1} & D_{1,2} \\ conjugate(D_{1,2}) & D_{2,2}\end{bmatrix}\right):$$

Example 1: free particle classical Boltzmann state

$$ExampleFreeParticle := \left\{\Upsilon_1 = \frac{1}{\sqrt{2}\cdot\sqrt[4]{\frac{2\cdot \mathrm{Pi}}{\beta}}}\cdot\exp\left(-\beta\cdot\frac{p^2}{4} + \frac{I\cdot p\cdot q}{2\cdot\hbar}\right), \Upsilon_2 = 0\right\}$$

$$ExampleFreeParticle := \left\{Upsi_1 = \frac{2^{1/4}\,e^{-\frac{\beta p^2}{4} + \frac{I p q}{2\hbar}}}{2\left(\frac{\pi}{\beta}\right)^{1/4}}, Upsi_2 = 0\right\} \quad \textbf{(3.1.1)}$$

Get the hybrid density matrix

$$simplify\left(eval\left(\left[\begin{array}{cc} D_{1,1} & D_{1,2} \\ conjugate(D_{1,2}) & D_{2,2} \end{array}\right], ExampleFreeParticle\right)\right) \text{ assuming } p :: \mathbb{R}, q :: \mathbb{R}, \hbar > 0, \beta > 0$$

$$\left[\begin{array}{cc} \frac{\sqrt{2}\sqrt{\beta}\, e^{-\frac{\beta p^2}{2}}}{2\sqrt{\pi}} & 0 \\ 0 & 0 \end{array}\right] \quad \textbf{(3.1.2)}$$

Example 2: harmonic oscillator classical Boltzmann state

$$H_0 := \frac{p^2}{2 \cdot m} + \frac{m \cdot \omega^2 \cdot q^2}{2} :$$

$$ExampleHarmonicOscillator := \left\{ \Upsilon_1 = \frac{\sqrt{\frac{\omega}{2 \cdot \mathrm{Pi} \cdot \beta}}}{H_0} \cdot \sqrt{1 - (1 + \beta \cdot H_0) \cdot \exp(-\beta \cdot H_0)}, \Upsilon_2 = 0 \right\} :$$

Solving the special case of a classical harmonic oscillator quadratically coupled to a degenerate two-level quantum system

Analytically derived exact solution

Take the random unitary matrix U

$$\#RandM := Matrix((i, j) \rightarrow rand(\,), 2, 2) :$$

$$\#U := simplify\left(LinearAlgebra\text{:-}MatrixExponential\left(\frac{I\cdot\left(RandM + RandM^{*}\right)}{rand(\ )}\right)\right):$$

Example from the paper

$$U := \begin{bmatrix} \frac{1}{2}\sqrt{2} & \frac{1}{2}\sqrt{2} \\ -\frac{1}{2}\sqrt{2} & \frac{1}{2}\sqrt{2} \end{bmatrix}:$$

Coupling term

$$\boldsymbol{\alpha\sigma} := simplify\left(\lambda\cdot U^{*}.\sigma_3\cdot U\right):$$

Construct the Hybrid equation to be solved

$$HarmonicOscEq := eval\left(HybridEq, \left\{H = H_0, f_1 = \frac{q^2}{2}\cdot\frac{Trace\left(\boldsymbol{\alpha\sigma}.\sigma_1\right)}{2}, f_2 = \frac{q^2}{2}\cdot\frac{Trace\left(\boldsymbol{\alpha\sigma}.\sigma_2\right)}{2}, f_3 = \frac{q^2}{2}\cdot\frac{Trace\left(\boldsymbol{\alpha\sigma}.\sigma_3\right)}{2}\right\}\right):$$

Introducing notations

$$\omega_{+} := \sqrt{\omega^2 + \frac{\lambda}{m}} : \omega_{-} := \sqrt{\omega^2 - \frac{\lambda}{m}} :$$

In the following exact solution, F_1 : and F_2 : denotes for the initial condition for Υ :

$$\left(subs\left(t = 0, \Upsilon_1\right) = F_1(q,p), subs\left(t = 0, \Upsilon_2\right) = F_2(q,p)\right):$$

$$\#y := (\Omega) \rightarrow U.\begin{bmatrix} F_1(q,p) \\ F_2(q,p) \end{bmatrix}$$

$$\Big|_{q = q\cdot\cos(\Omega\cdot t) - \frac{p\cdot\sin(\Omega\cdot t)}{m\cdot\Omega},\ p = p\cdot\cos(\Omega\cdot t) + m\cdot\Omega\cdot q\cdot\sin(\Omega\cdot t)} :$$

Using initial condition from the paper

$$y := (\Omega) \rightarrow U.\begin{bmatrix} \frac{\sqrt{\frac{\omega}{2\cdot\mathrm{Pi}\cdot\beta}}}{H_0}\cdot\sqrt{1 - \left(1 + \beta\cdot H_0\right)\cdot\exp\left(-\beta\cdot H_0\right)} \\ 0 \end{bmatrix}$$

$$q = q\cdot\cos(\Omega\cdot t) - \frac{p\cdot\sin(\Omega\cdot t)}{m\cdot\Omega}, p = p\cdot\cos(\Omega\cdot t) + m\cdot\Omega\cdot q\cdot\sin(\Omega\cdot t) :$$

Here is the sought exact solution

$$Y := U^{*}.\begin{bmatrix} y(\omega_{+})_{1} \\ y(\omega_{-})_{2} \end{bmatrix} :$$

$$ExSolution := \{\Upsilon_{1} = Y_{1}, \Upsilon_{2} = Y_{2}\} :$$

Verifying the initial conditions

$$\#simplify\left(eval\left(eval\left(\Upsilon_{1}, ExSolution\right), t=0\right) - F_{1}(q,p)\right)$$
$$\#simplify\left(eval\left(eval\left(\Upsilon_{2}, ExSolution\right), t=0\right) - F_{2}(q,p)\right)$$

Verifying the exact solution

$$\#simplify(combine(pdetest(ExSolution, HarmonicOscEq)))$$

Exact solution of Aleksandrov–Gerasimenko equation

Defyning equation

$$PoissonBracket := (f,g) \rightarrow \frac{\partial}{\partial q}(f).\frac{\partial}{\partial p}(g) - \frac{\partial}{\partial p}(f).\frac{\partial}{\partial q}(g) :$$

$$AleksandrovGerasimenkoEq := (DM, H) \rightarrow -\frac{\partial}{\partial t}(DM) - \frac{I}{\hbar}\cdot(H \bullet DM - DM \bullet H) + \frac{1}{2}\cdot PoissonBracket(H, DM) - \frac{1}{2}\cdot PoissonBracket(DM, H) :$$

Generic Initial condition

$$\#InitDM := \begin{bmatrix} c_{1,1}(q,p) & c_{1,2}(q,p) \\ c_{2,1}(q,p) & c_{2,2}(q,p) \end{bmatrix} :$$

Initial condition from the paper

$$InitDM := \begin{bmatrix} \frac{\omega\cdot\beta}{2\cdot\pi}\cdot\exp(-\beta\cdot H_0) & 0 \\ 0 & 0 \end{bmatrix}:$$

$$d := (\Omega) \rightarrow (U \bullet InitDM \bullet U^{*})$$

$$\Big|_{q = q\cdot\cos(\Omega\cdot t) - \frac{p\cdot\sin(\Omega\cdot t)}{m\cdot\Omega},\, p = p\cdot\cos(\Omega\cdot t) + m\cdot\Omega\cdot q\cdot\sin(\Omega\cdot t)} :$$

$$\varphi := \frac{\lambda}{2\cdot m\cdot\hbar\cdot\omega^3}\cdot\left(\frac{p^2 - (m\cdot\omega\cdot q)^2}{2\cdot m}\cdot\sin(2\cdot\omega\cdot t) - \omega\cdot\left(2\cdot t\cdot H_0 + p\cdot q\cdot(\cos(2\cdot\omega\cdot t) - 1)\right)\right):$$

$$DM := U^{*}.\begin{bmatrix} d(\omega_+)_{1,1} & e^{I\cdot\varphi}\cdot d(\omega)_{1,2} \\ e^{-I\cdot\varphi}\cdot d(\omega)_{2,1} & d(\omega_-)_{2,2} \end{bmatrix}\bullet U:$$

Testing initial condition

$$simplify(eval(DM, t = 0) - InitDM)$$

Testing the full solution

$$\#simplify\left(combine\left(AleksandrovGerasimenkoEq\left(DM, H_0 + \frac{q^2}{2}\cdot\boldsymbol{\alpha\sigma}\right)\right)\right)$$

Solving Pauli equation and generating code

The exact solution to the Paul equation for an oscillator with frequency Ω and the initial quantum state is the ground state with frequency ω

$$PD := (\Omega) \rightarrow \frac{\sqrt{\Omega}\,\sqrt{-I}\,m^{1/4}\,\omega^{1/4}\,e^{-\frac{\Omega\, m\, q^2\,(\cos(\Omega\, t)\,\omega\, I - \sin(\Omega\, t)\,\Omega)}{2\,\hbar\,(\Omega\cos(\Omega\, t)\, I - \omega\sin(\Omega\, t))}}}{\hbar^{1/4}\,\pi^{1/4}\,\sqrt{-I\,\Omega\cos(\Omega\, t) + \omega\sin(\Omega\, t)}}:$$

$$\psi := U^{*}.\begin{bmatrix} U_{1,1}\cdot PD(\omega_+) \\ U_{2,1}\cdot PD(\omega_-) \end{bmatrix}:$$

Perform the Wigner transform

$PauliParams := \left\{\hbar = 1, m = 1, \omega = 1\ , \lambda = \frac{95}{100}\right\}:$

$$WignerPD := (\Omega) \rightarrow \frac{1}{\pi} \cdot \int_{-\infty}^{+\infty} eval(eval(subs(I = -I, PD(\Omega)), PauliParams), q = q + s) \cdot eval(eval(PD(\Omega), PauliParams), q = q - s) \cdot \exp(2 \cdot I \cdot p \cdot s) \mathrm{d}s :$$

$TotalWigner := simplify\left(\left|U_{1,\,1}\right|^2 \cdot WignerPD(\omega_+) + \left|U_{2,\,1}\right|^2 \cdot WignerPD(\omega_-)\right)$assuming $t > 0$:

Get code for the Wigner function

$CodeGeneration{:}\text{-}Python(TotalWigner, optimize, resultname = 'W')$

$$\begin{bmatrix} \int_{-\infty}^{+\infty} \left|U_{1,\,1} \cdot PD(\omega_{`+`})\right|^2 \Big|_{PauliParams} \mathrm{d}q & 0 \\ 0 & \int_{-\infty}^{+\infty} \left|U_{2,\,1} \cdot PD(\omega_-)\right|^2 \Big|_{PauliParams} \mathrm{d}q \end{bmatrix} \text{assuming } q :: \mathbb{R}, t > 0$$

$$rho\_12 := simplify\left(\int_{-\infty}^{+\infty} simplify\left(eval\left(U_{1,\,1} \cdot PD(\omega_{`+`}) \cdot conjugate\left(U_{2,\,1} \cdot PD(\omega_-)\right), PauliParams\right)\right) \mathrm{d}q\right) \text{assuming } q :: \mathbb{R}, t > 0 :$$

$CodeGeneration{:}\text{-}Python(rho\_12\ , optimize, resultname = 'rotated\_rho\_12')$

$$simplify\left(\int_{-\infty}^{+\infty} \left|U_{1,\,1} \cdot PD(\omega_{`+`})\right|^2 \Big|_{PauliParams} \mathrm{d}q\right) \text{assuming } q :: \mathbb{R}, t > 0$$

$$simplify\left(\int_{-\infty}^{+\infty} \left|U_{2,\,1} \cdot PD(\omega_-)\right|^2 \Big|_{PauliParams} \mathrm{d}q\right) \text{assuming } q :: \mathbb{R}, t > 0$$

$plot(\mathrm{Re}(rho\_12), t = 0\,..4)$

$plot(\mathrm{Im}(rho\_12), t = 0\,..4)$

Code generation for illustration

Specify the initial condition - the same as in Example 2: harmonic oscillator classical Boltzmann state

$$\#F_1 := (q,p) \rightarrow \frac{\sqrt{\frac{\omega}{2 \cdot \mathrm{Pi} \cdot \beta}}}{H_0} \cdot \sqrt{1 - \left(1 + \beta \cdot H_0\right) \cdot \exp\left(-\beta \cdot H_0\right)} :$$

$$\#F_2 := (q,p) \rightarrow 0 :$$

$ParamsToPlot := \{\hbar = 1, m = 1, \} :$

$SolutionToPlot := eval(ExSolution, ParamsToPlot) :$

One more (redundant) check that the obtain solution satisfies the equation

$pdetest(SolutionToPlot, eval(HarmonicOscEq, ParamsToPlot))$ assuming $\beta > 0, \omega > 0$

$CodeGeneration{:}\text{-}Python\left(eval\left(eval\left(\mathrm{D}_{1,1}, SolutionToPlot\right), ParamsToPlot\right), optimize, resultname = \text{"\_D11"}\right)$ assuming $p :: \mathbb{R}, q :: \mathbb{R}, \beta > 0, \omega > 0$

$CodeGeneration{:}\text{-}Python\left(eval\left(eval\left(\mathrm{D}_{1,2}, SolutionToPlot\right), ParamsToPlot\right), optimize, resultname = \text{"\_D12"}\right)$ assuming $p :: \mathbb{R}, q :: \mathbb{R}, \beta > 0, \omega > 0$

$CodeGeneration{:}\text{-}Python\left(eval\left(eval\left(\mathrm{D}_{2,2}, SolutionToPlot\right), ParamsToPlot\right), optimize, resultname = \text{"\_D22"}\right)$ assuming $p :: \mathbb{R}, q :: \mathbb{R}, \beta > 0, \omega > 0$

Code for plotting the solution for Aleksandrov–Gerasimenko equation

Specify the initial condition - the same as in Example 2: harmonic oscillator classical Boltzmann state

$$\#c_{1,1}(q,p) := \frac{\omega \cdot \beta}{2 \cdot \pi} \cdot \exp\left(-\beta \cdot H_0\right) :$$

$$\#c_{1,2}(q,p) := 0 :$$

$$\#c_{2,1}(q,p) := 0 :$$

$$\#c_{2,2}(q,p) := 0 :$$

Check the normalization

$int\left(c_{1,1}(q,p), [q = -\infty .. +\infty, p = -\infty .. +\infty]\right)$ assuming $\beta > 0, m > 0, \omega > 0$

$CodeGeneration{:-}Python(simplify(eval(DM[1, 1], ParamsToPlot)), optimize, resultname = "\_D11")$ assuming $p :: \mathbb{R}, q :: \mathbb{R}, \beta > 0, \omega > 0$

$CodeGeneration{:-}Python(simplify(eval(DM[1, 2], ParamsToPlot)), optimize, resultname = "\_D12")$ assuming $p :: \mathbb{R}, q :: \mathbb{R}, \beta > 0, \omega > 0$

$CodeGeneration{:-}Python(simplify(eval(DM[2, 2], ParamsToPlot)), optimize, resultname = "\_D22")$ assuming $p :: \mathbb{R}, q :: \mathbb{R}, \beta > 0, \omega > 0$