

# Simulating bipartite quantum systems

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We are interested in numerical simulations of the behaviour of various types of bipartite quantum systems with a focus on the behaviour of the entanglement entropy.

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## I. COLLISION BETWEEN A PROJECTILE AND A DIATOMIC MOLECULE

### A. Hamiltonian and Schrödinger equation

We consider a system described by a classical Hamiltonian

$$\mathcal{H} = \hbar\omega \left( \frac{p_x^2}{2m_1} + \frac{1}{2}m_1x^2 + \frac{p_y^2}{2m_2} + \lambda e^{x-y} \right), \quad (1)$$

where  $(x, p_x)$  and  $(y, p_y)$  are canonically conjugate pairs, respectively. All quantities within the round brackets are dimensionless, while  $\omega$  is a frequency with dimensions of inverse time. Upon quantization, we may re-write the Hamiltonian as

$$\hat{H} = \hbar\omega(\hat{H}_1 + \hat{H}_2 + \lambda\hat{V}_1\hat{V}_2), \quad (2)$$

with

$$\hat{H}_1 = \frac{\hat{p}_x^2}{2m_1} + \frac{1}{2}m_1\hat{x}^2, \quad \hat{H}_2 = \frac{\hat{p}_y^2}{2m_2}, \quad \hat{V}_1 = e^{\hat{x}}, \quad \hat{V}_2 = e^{-\hat{y}}. \quad (3)$$

Physically, this system represents a diatomic molecule (subsystem 1) and a projectile (subsystem 2). The  $x$  coordinate represents the separation between the two atoms in the molecule, while  $y$  represents the separation between the projectile and the molecule.

We now use units in which  $\hbar = 1$ . Upon quantization, the Schrödinger equation for the system is

$$i\frac{\partial\psi}{\partial\tau} = -\frac{1}{2m_1}\frac{\partial^2\psi}{\partial x^2} + \frac{1}{2}m_1x^2\psi - \frac{1}{2m_2}\frac{\partial^2\psi}{\partial y^2} + \lambda e^{x-y}\psi, \quad (x, y) \in \mathbb{R}^2, \quad (4)$$

where  $\tau = \omega t$ .

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### B. Method of lines discretization and Crank-Nicholson stencil

In order to solve the Schrödinger equation numerically using the method of lines, we consider a finite computational domain and Dirichlet boundary conditions:

$$\Omega = \{(x, y) \in [-\frac{1}{2}L_1, \frac{1}{2}L_1] \times [-\frac{1}{2}L_2, \frac{1}{2}L_2]\}, \quad \psi|_{\partial\Omega} = 0. \quad (5)$$

Now, suppose that we discretize the  $x$  and  $y$  directions such that

$$x \mapsto \{x_0 = -\frac{1}{2}L_1, x_1, x_2 \dots x_n, x_{n+1} = \frac{1}{2}L_1\}, \quad x_{i+1} - x_i = h_x = L_1/(n+1), \quad (6)$$

$$y \mapsto \{y_0 = -\frac{1}{2}L_2, y_1, y_2 \dots y_m, y_{m+1} = \frac{1}{2}L_2\}, \quad y_{j+1} - y_j = h_y = L_2/(m+1). \quad (7)$$

The Dirichlet boundary conditions then read

$$\psi(\tau, x_0, y) = \psi(\tau, x_{n+1}, y) = \psi(\tau, x, y_0) = \psi(\tau, x, y_{m+1}) = 0. \quad (8)$$

We can define an  $n \times m$  matrix  $\Psi(\tau)$  whose entries are numeric approximations to  $\psi(\tau, x, y)$  evaluated at the interior  $xy$ -gridpoints

$$\Psi(\tau) \in \mathbb{C}^{n \times m}, \quad \Psi_{ij}(\tau) \approx \psi(\tau, x_i, y_j). \quad (9)$$

Then the Schrödinger equation may be approximated as

$$i \frac{d\Psi}{d\tau} = \frac{1}{2m_1} P_x^2 \Psi + \frac{1}{2m_2} \Psi P_y^2 + \frac{1}{2} m_1 X^2 \Psi + \lambda U_x \Psi U_y. \quad (10)$$

where  $H_x, X \in \mathbb{R}^{n \times n}$  and  $H_y, Y \in \mathbb{R}^{m \times m}$  such that

$$P_x^2 = -\frac{1}{h_x^2} \begin{pmatrix} -2 & 1 & & \\ 1 & -2 & 1 & \\ & 1 & -2 & 1 \\ & & \ddots & \ddots \end{pmatrix}, \quad P_y^2 = -\frac{1}{h_y^2} \begin{pmatrix} -2 & 1 & & \\ 1 & -2 & 1 & \\ & 1 & -2 & 1 \\ & & \ddots & \ddots \end{pmatrix},$$

$$X = \begin{pmatrix} x_1 & & & \\ & x_2 & & \\ & & \ddots & \\ & & & x_n \end{pmatrix}, \quad U_x = \begin{pmatrix} e^{x_1} & & & \\ & e^{x_2} & & \\ & & \ddots & \\ & & & e^{x_m} \end{pmatrix}, \quad U_y = \begin{pmatrix} e^{-y_1} & & & \\ & e^{-y_2} & & \\ & & \ddots & \\ & & & e^{-y_m} \end{pmatrix}. \quad (11)$$

This can be recast into the standard form for a system of  $n \times m$  of linear first order differential equations by defining the “vectorization”  $\vec{\Psi}$  of  $\Psi$ :

$$\vec{\Psi} = \text{vec}(\Psi). \quad (12)$$

Basically,  $\vec{\Psi}$  is the  $n \times m$  dimensional column vector formed by stacking the columns of  $\Psi$  on top of one another. Then, we have

$$\frac{d\vec{\Psi}}{d\tau} = A\vec{\Psi}, \quad (13)$$

where

$$A = -i \left[ \frac{1}{2m_1} (I_m \otimes P_x^2) + \frac{1}{2} m_1 (I_m \otimes X^2) + \frac{1}{2m_2} (P_y^2 \otimes I_n) + \lambda (U_y \otimes U_x) \right]. \quad (14)$$

Here,  $I_n$  and  $I_m$  are  $n$  and  $m$  dimensional identity matrices, respectively, and  $\otimes$  represents the matrix Kronecker product. (We have made use of the fact that all matrices are symmetric.) The matrix ODE can then be solved numerically by introducing a time discretization  $\tau \mapsto \{\tau_k\}$  with  $\tau_{k+1} - \tau_k = s$ . The Crank-Nicholson stencil for solving the system is then

$$(I_{nm} - \frac{1}{2}sA) \vec{\Psi}_{k+1} = (I_{nm} + \frac{1}{2}sA) \vec{\Psi}_k, \quad \vec{\Psi}(\tau_k) \approx \vec{\Psi}_k. \quad (15)$$

Suppose we want to calculate the expectation value of some phase space function of  $x$  and  $p(x)$ ; i.e.  $f(x, p_x)$ . Due to linearity, the action of the associated operator  $\hat{f}$  on the wavefunction will be approximated by a left-acting linear map on the  $\Psi$  matrix

$$(\hat{f}\psi)(\tau, x_i, y_j) \approx \sum_{i'} F_{ii'} \Psi_{i'j}, \quad (16)$$

for some matrix  $F$ . Hence, we can approximate the expectation value as

$$\langle f(x, p_x) \rangle = \iint dx dy \psi^*(\tau, x, y) (\hat{f}\psi)(\tau, x, y) \approx \sum_{ii'j} h_x h_y \Psi_{ij}^* F_{ii'} \Psi_{i'j} = \text{Tr} [\rho_1 F], \quad (17)$$

where the reduced density matrix for the  $x$ -sector is

$$\rho_1 = h_x h_y \Psi \Psi^\dagger. \quad (18)$$

Similarly, the reduced density matrix for the  $y$ -sector is

$$\rho_2 = h_x h_y \Psi^T \Psi^*. \quad (19)$$

Explicitly, expectation values and variances of  $x$  and  $y$  are given by

$$\langle x \rangle = \text{Tr} (\rho_1 X), \quad \text{Var}(x) = \sqrt{\text{Tr} (\rho_1 X^2) - \langle x \rangle^2}, \quad \langle y \rangle = \text{Tr} (\rho_2 Y), \quad \text{Var}(y) = \sqrt{\text{Tr} (\rho_2 Y^2) - \langle y \rangle^2} \quad (20)$$

Once we have the reduced density matrices, the von Neumann entanglement entropy can be obtained by calculating the eigenvalues  $\{\Lambda_i\}$  of either  $\rho_1$  or  $\rho_2$ , and then computing the sum

$$S_{\text{VN}} = - \sum_i \Lambda_i \ln \Lambda_i. \quad (21)$$

Note that since the density matrices are themselves functions of time, the above expectation values and entanglement entropy are also functions of time.

### C. Solution of the Schrödinger equation via subsystem Hamiltonian eigenbasis expansion

We assume that the energy eigenvalue problem for each of the subsystem Hamiltonians is easily solvable:

$$\hat{H}_1 |\mu\rangle = E_\mu |\mu\rangle, \quad \hat{H}_2 |\nu\rangle = E_\nu |\nu\rangle. \quad (22)$$

In this section, we work in a finite truncation where we keep the  $d_1$  and  $d_2$  lowest energy eigenstates of subsystem 1 (the oscillator) and subsystem 2 (the projectile), respectively. Our notation is such that the indices  $\mu, \mu' = 0, 1, 2 \dots d_1 - 1$  will always be associated with subsystem 1 and the indices  $\nu, \nu' = 1, 2 \dots d_2$  will always be associated with subsystem 2.<sup>1</sup> Then, a complete basis for the total Hilbert space is given by the  $d_1 \times d_2$  basis states

$$|\mu, \nu\rangle = |\mu\rangle \otimes |\nu\rangle, \quad \langle \mu', \nu' | \mu, \nu \rangle = \delta_{\mu\mu'} \delta_{\nu\nu'}. \quad (23)$$

We write the full state vector of the system in the Schrödinger representation as

$$|\psi(\tau)\rangle = \sum_{\mu\nu} z_{\mu,\nu}(\tau) |\mu, \nu\rangle. \quad (24)$$

Inserting this into the Schrödinger equation

$$i\partial_\tau |\psi(\tau)\rangle = \hat{H} |\psi(\tau)\rangle \quad (25)$$

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<sup>1</sup> The slightly odd indexing conventions for the two subsystems will be for later convenience.

yields

$$i\partial_\tau z_{\mu',\nu'}(\tau) = \sum_{\mu\nu} \langle \mu', \nu' | \hat{H} | \mu, \nu \rangle z_{\mu,\nu}(\tau). \quad (26)$$

We organize the expansion coefficients into a matrix:

$$Z(\tau) = \begin{pmatrix} z_{0,1}(\tau) & z_{0,2}(\tau) & \cdots & z_{0,d_2}(\tau) \\ z_{1,1}(\tau) & z_{1,2}(\tau) & \cdots & z_{1,d_2}(\tau) \\ \vdots & \vdots & \ddots & \vdots \\ z_{d_1-1,1}(\tau) & z_{d_1-1,2}(\tau) & \cdots & z_{d_1-1,d_2}(\tau) \end{pmatrix}.$$

Inserting the expansion (24) into the Schrodinger equation yields:

$$i\partial_\tau Z = H_1 Z + Z H_2 + \lambda V_1 Z V_2^\top, \quad (27)$$

where the  $H_1$ ,  $H_2$ ,  $V_1$ , and  $V_2$  square matrices have entries

$$\begin{aligned} (H_1)_{\mu'\mu} &= \langle \mu' | \hat{H}_1 | \mu \rangle, & (V_1)_{\mu'\mu} &= \langle \mu' | \hat{V}_1 | \mu \rangle, \\ (H_2)_{\nu'\nu} &= \langle \nu' | \hat{H}_2 | \nu \rangle, & (V_2)_{\nu'\nu} &= \langle \nu' | \hat{V}_2 | \nu \rangle. \end{aligned} \quad (28)$$

Note that since  $|\mu\rangle$  and  $|\nu\rangle$  are eigenvectors of  $\hat{H}_1$  and  $\hat{H}_2$ , respectively,  $H_1$  and  $H_2$  are real diagonal matrices. Furthermore,  $V_1$  and  $V_2$  are Hermitian matrices due to the self-adjointness of the associated operators. Equation (27) represents  $d_1 \times d_2$  complex linear differential equations whose solutions completely specify the quantum dynamics of the system. In addition to the above, other useful matrices are the representations of  $\hat{x}$ ,  $\hat{x}^2$ , etc., in the respective eigenbases of  $\hat{H}_1$ , and  $\hat{H}_2$ . These will have matrix elements of the form

$$\begin{aligned} (X^k)_{\mu'\mu} &= \langle \mu' | \hat{x}^k | \mu \rangle, & (P_x^k)_{\mu'\mu} &= \langle \mu' | \hat{p}_x^k | \mu \rangle, \\ (Y^k)_{\nu'\nu} &= \langle \nu' | \hat{y}^k | \nu \rangle, & (P_y^k)_{\nu'\nu} &= \langle \nu' | \hat{p}_y^k | \nu \rangle. \end{aligned} \quad (29)$$

with  $k = 1, 2, \dots$

For the oscillator, the energy eigenvectors are the familiar Fock states for the simple harmonic oscillator. It is useful to define raising and lowering operators by

$$\hat{a} = \frac{m_1^{1/2} \hat{x} + i m_1^{-1/2} \hat{p}}{\sqrt{2}}, \quad \hat{a}^\dagger = \frac{m_1^{1/2} \hat{x} - i m_1^{-1/2} \hat{p}}{\sqrt{2}} \quad (30)$$

which implies that

$$[\hat{a}, \hat{a}^\dagger] = 1, \quad \hat{H}_1 = \hat{a}^\dagger \hat{a} + \frac{1}{2}. \quad (31)$$

Hamiltonian eigenstates satisfy

$$\hat{H}_1 |\mu\rangle = (\mu + \frac{1}{2}) |\mu\rangle, \quad \mu = 0, 1, 2, \dots \quad (32)$$

The coordinate representation of the eigenfunctions is

$$\chi_\mu(x) = \langle x | \mu \rangle = \frac{1}{\sqrt{2^\mu \mu!}} \left( \frac{m_1}{\pi} \right)^{1/4} e^{-m_1 x^2/2} H_\mu(\sqrt{m_1} x), \quad (33)$$

where  $H_\mu$  is a Hermite polynomial. From this we can obtain

$$X = \frac{1}{\sqrt{2m_1}} \begin{pmatrix} 0 & \sqrt{1} & & \\ \sqrt{1} & 0 & \sqrt{2} & \\ & \sqrt{2} & 0 & \\ & & \ddots & \ddots \end{pmatrix}, \quad P = -i\sqrt{\frac{m_1}{2}} \begin{pmatrix} 0 & +\sqrt{1} & & \\ -\sqrt{1} & 0 & +\sqrt{2} & \\ & -\sqrt{2} & 0 & \\ & & \ddots & \ddots \end{pmatrix}, \quad H_1 - \frac{1}{2}I = \begin{pmatrix} 0 & & & \\ & 1 & & \\ & & 2 & \\ & & & \ddots \end{pmatrix}, \quad (34)$$

and  $I$  is the identity matrix. The  $V_1$  matrix can be shown to have elements

$$(V_1)_{\mu\mu'} = (V_1)_{\mu'\mu} = e^{1/4 m_1} (2m_1)^{-(\mu-\mu')/2} \sqrt{\frac{\mu'!}{\mu!}} L_{\mu'}^{\mu-\mu'} \left( -\frac{1}{2m_1} \right), \quad \mu \geq \mu', \quad (35)$$

where  $L_{\mu'}^{\mu-\mu'}$  are generalized Laguerre polynomials.

For the projectile, the above matrix elements can be written out explicitly if we note that a complete basis of eigenfunctions (written in the standard coordinate representation is):

$$\phi_\nu(y) = \langle y|\nu\rangle = \sqrt{\frac{2}{L_2}} \sin\left[\frac{\nu\pi}{2}\left(\frac{2y}{L_2} + 1\right)\right]. \quad (36)$$

We then have

$$\begin{aligned} (H_2)_{\nu'\nu} &= \frac{\nu^2\pi^2}{2m_2L_2^2}\delta_{\nu\nu'}, & (V_2)_{\nu'\nu} &= \frac{4\pi^2L_2\nu\nu'[e^{L_2/2} - (-1)^{\nu+\nu'}e^{-L_2/2}]}{[L_2^2 + \pi^2(\nu + \nu')^2][L_2^2 + \pi^2(\nu - \nu')^2]}, \\ (Y)_{\nu'\nu} &= \begin{cases} \frac{4L_2\nu\nu'[(-1)^{\nu+\nu'} - 1]}{\pi^2(\nu - \nu')^2(\nu + \nu')^2} & \text{for } \nu \neq \nu', \\ 0 & \text{for } \nu = \nu', \end{cases} & (P_y)_{\nu'\nu} &= \begin{cases} i\frac{2\nu\nu'[(-1)^{\nu+\nu'} - 1]}{L_2(\nu'^2 - \nu^2)} & \text{for } \nu \neq \nu', \\ 0 & \text{for } \nu = \nu', \end{cases} \\ (Y^2)_{\nu'\nu} &= \begin{cases} \frac{4L_2^2\nu\nu'[(-1)^{\nu+\nu'} + 1]}{\pi^2(\nu - \nu')^2(\nu + \nu')^2} & \text{for } \nu \neq \nu', \\ \frac{L_2^2(\pi^2\nu^2 - 6)}{12\nu^2\pi^2} & \text{for } \nu = \nu', \end{cases} & (P_y^2)_{\nu'\nu} &= \frac{\nu^2\pi^2}{L_2^2}\delta_{\nu\nu'}. \end{aligned}$$

## II. TEST CASE

A suitable test case for both the Crank-Nicholson method and the eigenbasis expansion method involves real space initial data for the wavefunction to be a product of the ground state oscillator wavefunction times a Gaussian wavepacket for the projectile with initial position and velocity  $y_0$  and  $p_0$ , respectively.

$$\psi(0, x, y) = \mathcal{N}\chi_0(x)e^{ip_0y} \exp\left[-\frac{(y - y_0)^2}{4\sigma^2}\right], \quad (37)$$

where

$$\chi_0(x) = \frac{m_1^{1/4}}{\pi^{1/4}} e^{-m_1x^2/2}, \quad (38)$$

and  $\mathcal{N}$  is a normalization factor

$$\mathcal{N} = \left\{ \int_{-L_2}^{L_2} dy \exp\left[-\frac{(y - y_0)^2}{2\sigma^2}\right] \right\}^{-1/2}, \quad (39)$$

which could be expressed in terms of an error function if desired. For the eigenbasis method, initial data for  $z_{\mu\nu}$  will be

$$z_{\mu\nu}(0) = \delta_{\mu,0}c_\nu, \quad c_\nu = \mathcal{N}\sqrt{\frac{2}{L_2}} \int_{-L_2}^{L_2} dy \sin\left[\frac{\nu\pi}{2}\left(\frac{2y}{L_2} + 1\right)\right] e^{ip_0y} \exp\left[-\frac{(y - y_0)^2}{4\sigma^2}\right]. \quad (40)$$

For the test case, we will take parameters

$$\lambda = 1, \quad m_1 = 1, \quad m_2 = 1, \quad y_0 = 10, \quad p_0 = -1, \quad \sigma = 3. \quad (41)$$

These parameters are fundamental, but there are additional “nuisance” parameters that must be selected in order for either numerical scheme to run. Some suggested values are

$$L_1 = 10, \quad L_2 = 50, \quad d_1 = 10, \quad d_2 = 40, \quad \tau \in [0, 20]. \quad (42)$$

It may be necessary to adjust these to get reasonable results.

### III. PLOTS FROM DOYEON

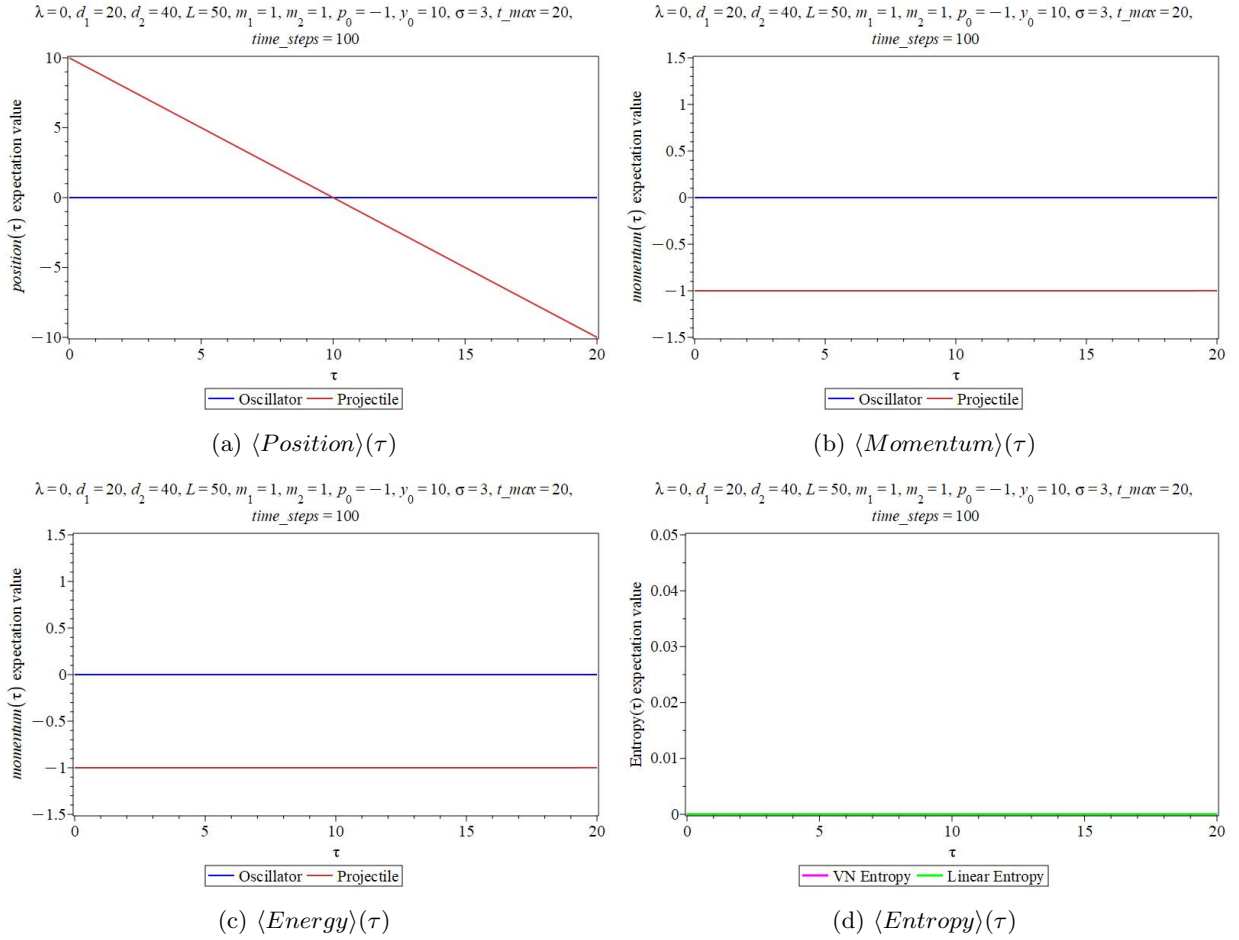
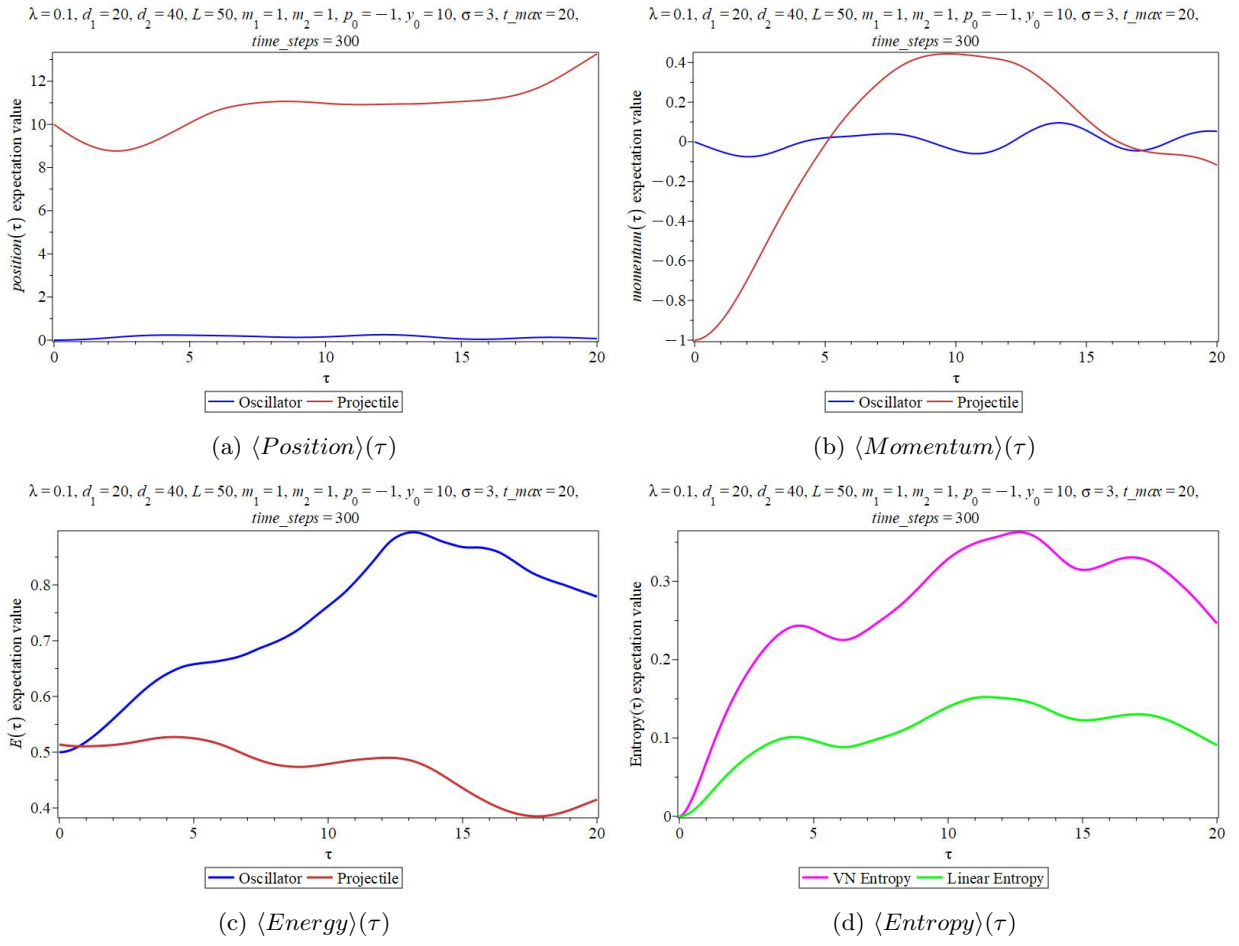
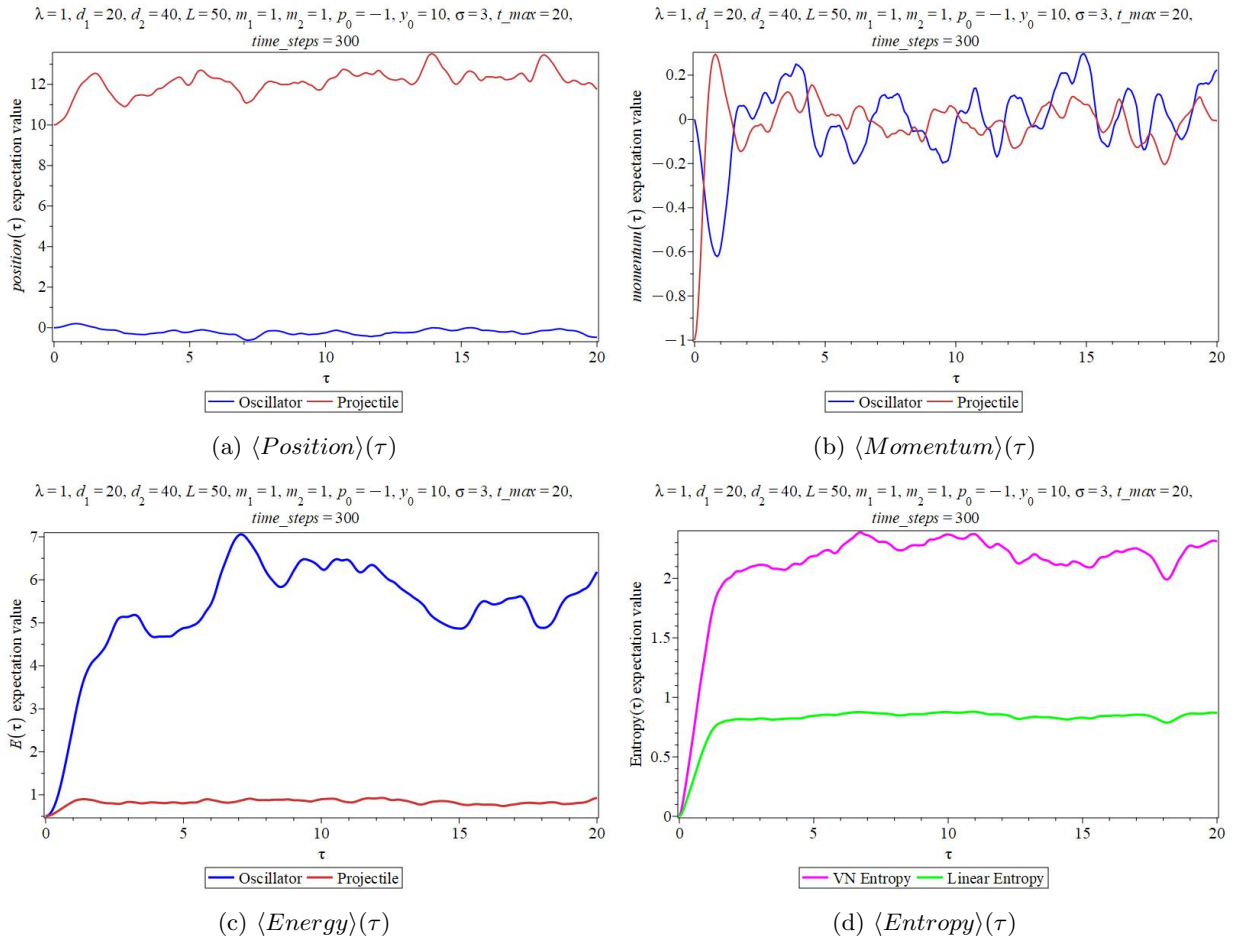


FIG. 1:  $\lambda = 0, y_0 = 10$

FIG. 2:  $\lambda = 0.1, y_0 = 10$

FIG. 3:  $\lambda = 1, y_0 = 10$



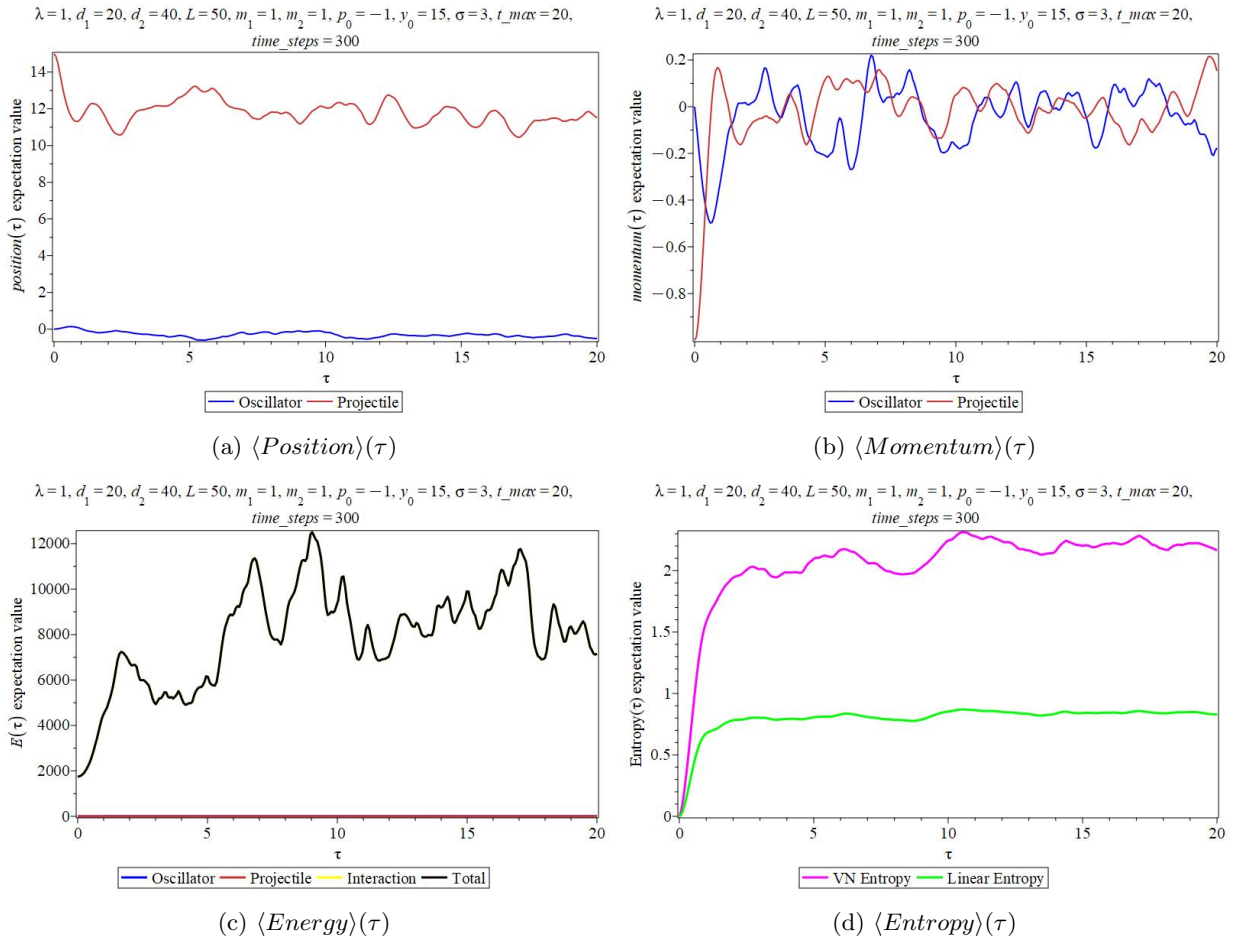
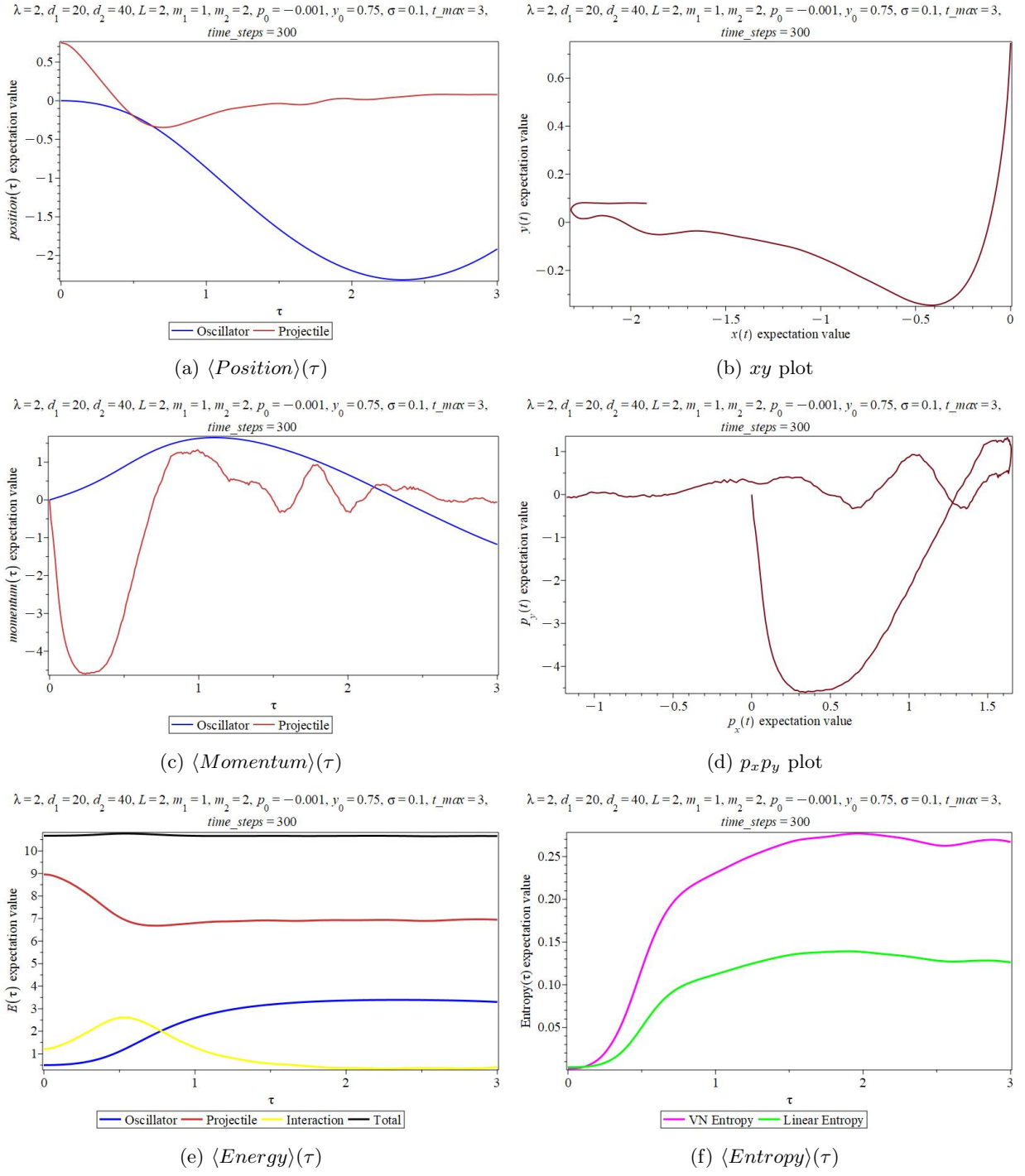
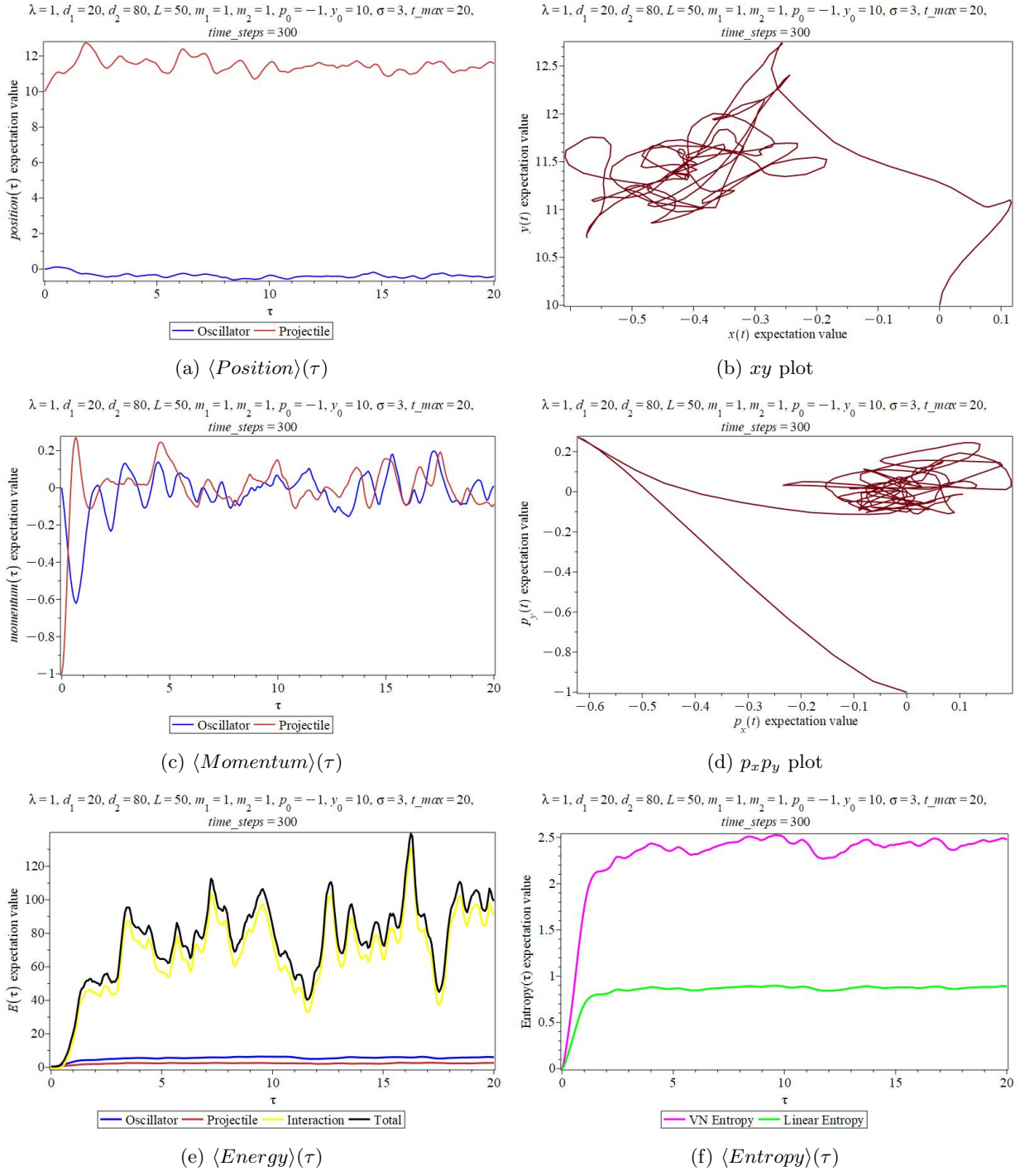
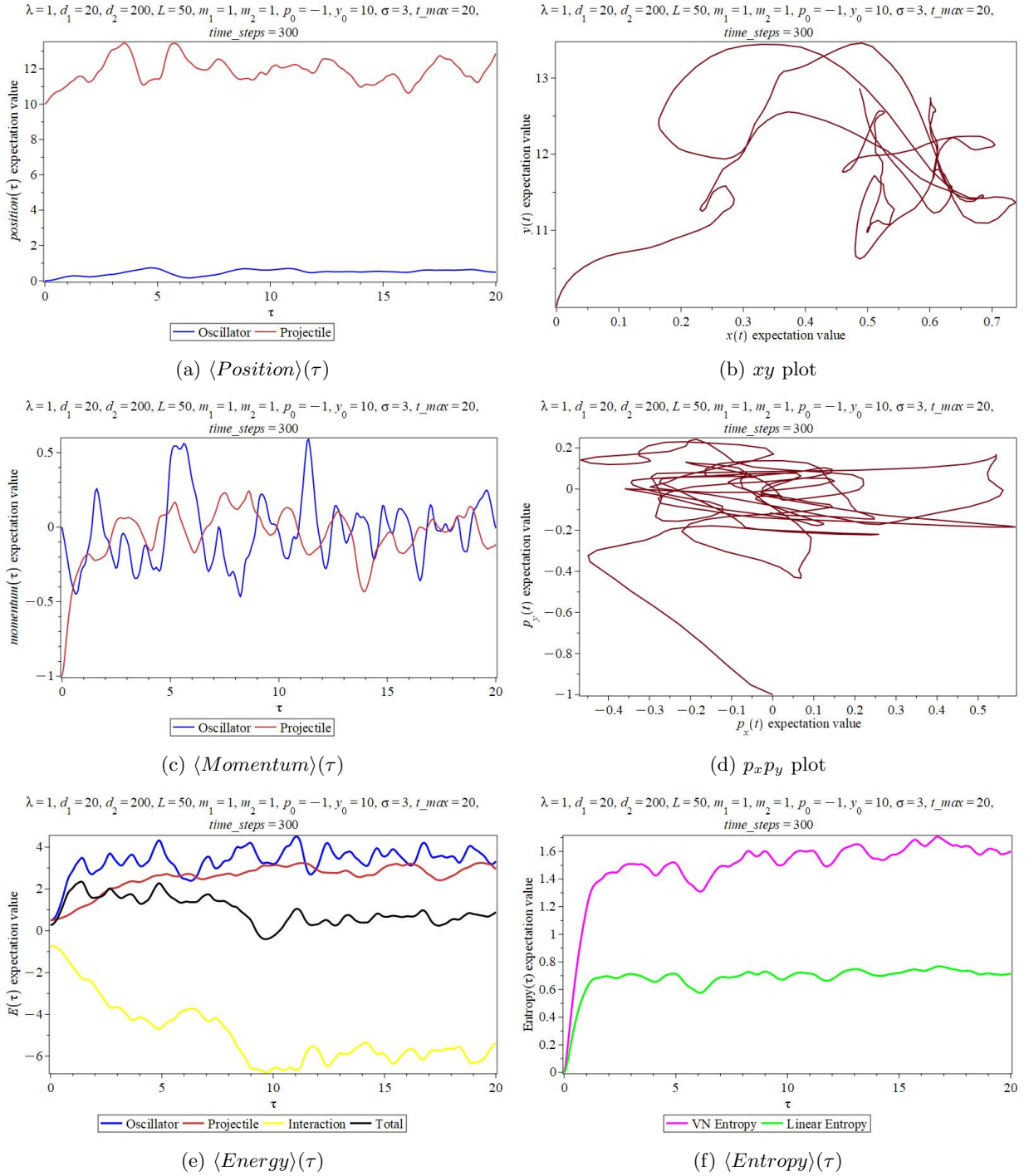


FIG. 4:  $\lambda = 1, y_0 = 15$ , in (c) the yellow line(/the red line) overlapped in the black line(/the blue line)

FIG. 5:  $L = 2$

FIG. 6:  $d_2 = 80$

FIG. 7:  $d_2 = 200$ 

#### IV. PLOTS FROM GAIA

##### A. Introduction

This section shall be a working section to include any plots and work that I do over time. This will all be produced using either the main Python file on the Digital Research Alliance of Canada, or locally through a Jupyter (ipynb) notebook. All of this code will align with a public GitHub that I will update regularly. **This GitHub also includes videos for everything here, showing the wave evolution.** It can be found at the following address:

[https://github.com/gaianoseworthy/CN\\_Schrodinger](https://github.com/gaianoseworthy/CN_Schrodinger).

Furthermore, whenever the Hamiltonian is calculated, it is done so using the following method:

```
1 X2 = np.diag(np.vectorize(lambda x : x**2)(x))
2 Px = (-1/(hbar**2))*sps.diags([1, -2, 1], [-1, 0, 1], shape=(n, n))
3 HPx = (1/(2*1)) * (Px**2) + (1/)*X2
4 observables[i,3] = np.real(np.trace(np.matmul(HPx, rho1)))
```

## B. Ground State 100x5000x1000

In this section, and really all future sections, the initial wavefunction will be set to avoid the extreme oscillations initially. The wavefunction is:

$$\Psi_0(x, y, t) = e^{-i(v_x x - v_y y)} e^{-\frac{(y-y_0)^2}{4\sigma_y^2}} \frac{1}{\sqrt{2\pi^4}} e^{-\frac{x^2}{2}}$$

It will also use the following initial variables:

- $x \in [-10, 10], m = 100$
- $y \in [-10, 90], n = 500$
- $t \in [0, 250], N = 1000$
- $x_0 = 0, y_0 = 75$
- $v_x = 0, v_y = -1$
- $\sigma_y = 1$
- $\lambda = 1$

This produces the following result:

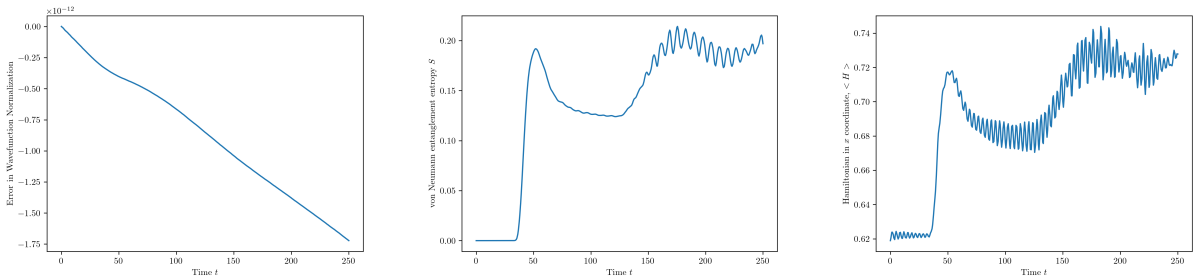


FIG. 8: Normalization, Entropy, and Hamiltonian of the 100x5000x1000 test with non-ground state initial Gaussian conditions.

## C. Low Lambda 100x5000x2000

Another interesting question is what if we set *lambda* to some low number, such as 0.01, with the new ground state wavefunction? Well, these results are as follows:

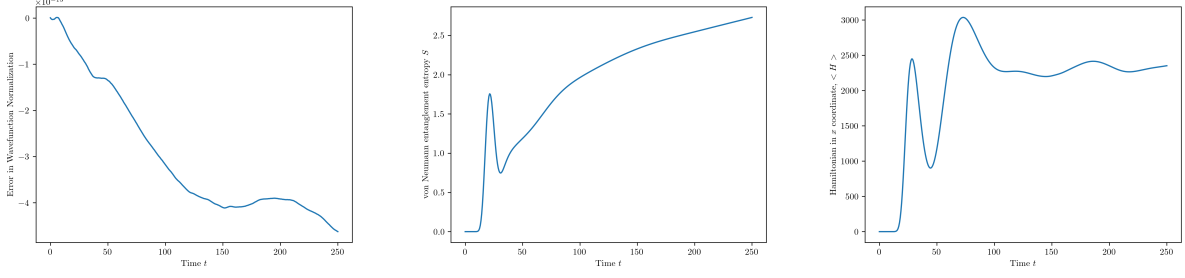


FIG. 9: Normalization, Entropy, and Hamiltonian of the 100x5000x1000 test with non-ground state initial Gaussian conditions.

#### D. Meeting Variables

For this section, I will use a series of variables agreed upon in the June 11 meeting, those being:

- $x \in [-5, 5], m = 100$
- $y \in [-25, 25], n = 5000$
- $t \in [0, 100], N = 1000$
- $x_0 = 0, y_0 = 10$
- $v_x = 0, v_y = -1$
- $\sigma_y = 3$
- $\lambda = 1$

This produced the following graphs:

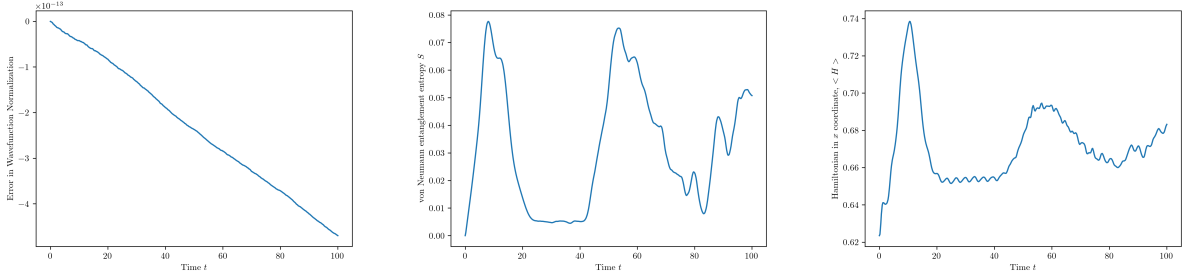


FIG. 10: Normalization, Entropy, and Hamiltonian of the 100x5000x1000 test with ground-state initial conditions and meeting-agreed-upon parameters.

The actual behaviour of the wave can be best described as a slow reflection upon the  $y = 0$  point, then later a reflection upon the top of the boundary, and finally another reflection upon the  $y = 0$  point. The jumps in entropy both happen at the reflection upon  $y = 0$ .

#### E. Expected Value Test 100x500x1000

The following results are similar to those above, as follows:

- $x \in [-5, 5], m = 100$
- $y \in [-5, 45], n = 500$

- $t \in [0, 40], N = 1000$

- $x_0 = 0, y_0 = 20$

- $v_x = 0, v_y = -1$

- $\sigma_y = 3$

- $\lambda = 1$

For the usual 3 plots, we get

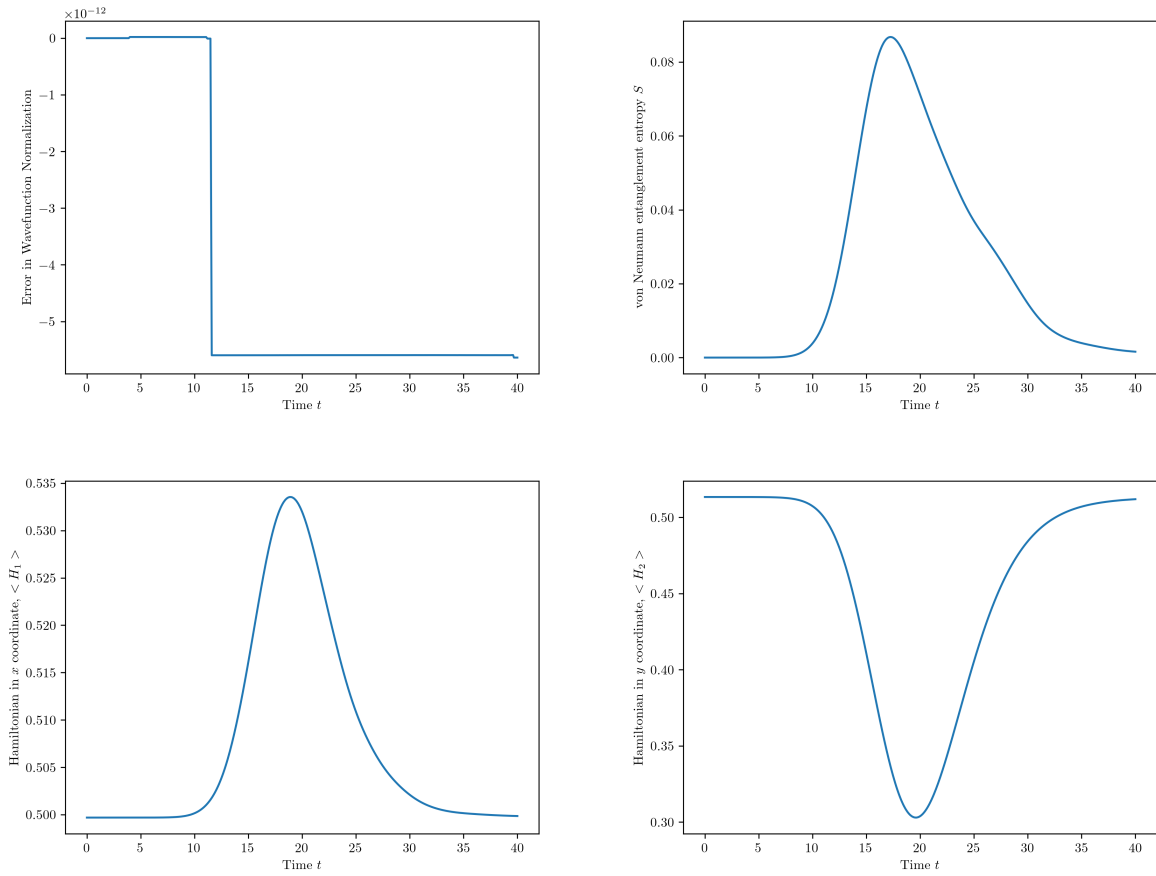


FIG. 11: Normalization, Entropy, and the  $x$  and  $y$  Hamiltonians respectively of the 100x500x1000 test with ground-state initial conditions and parameters above.

Furthermore, this gives the following expected values for  $\langle x \rangle$  and  $\langle y \rangle$ :

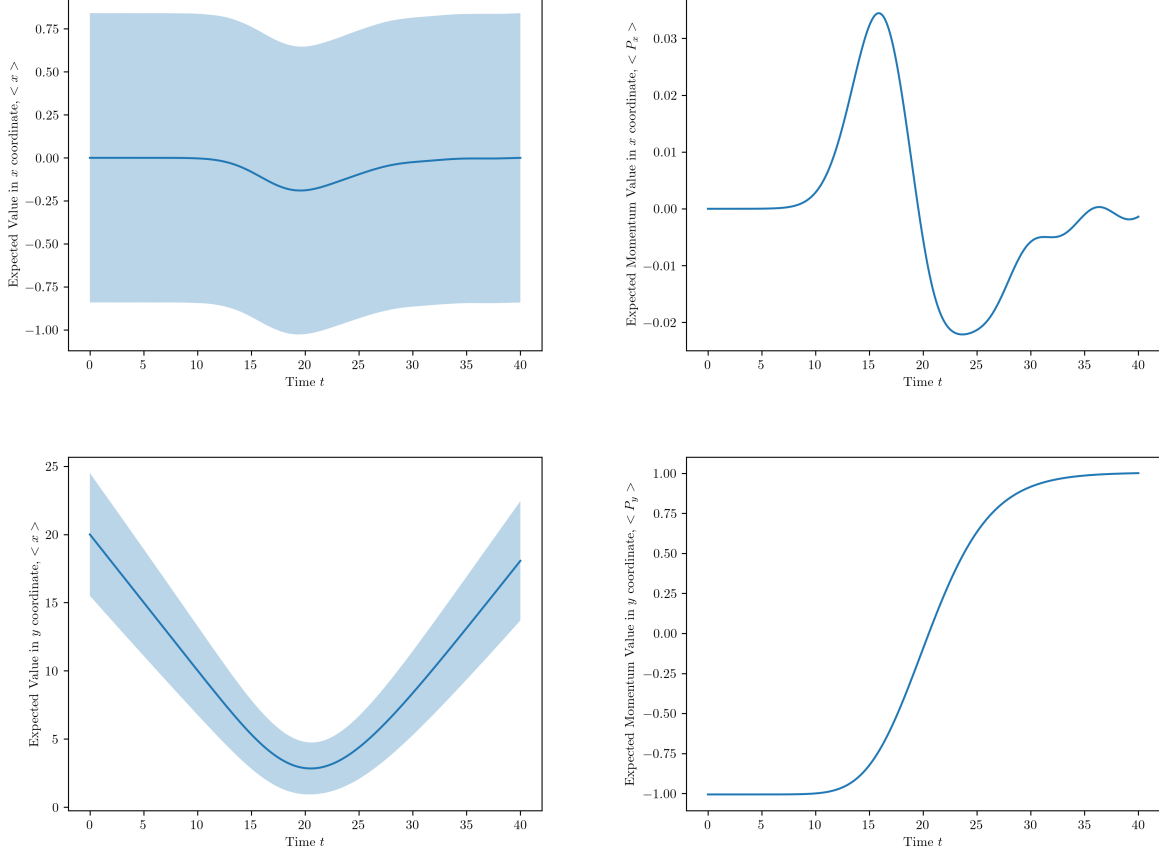


FIG. 12: Expected values for  $x$ ,  $p_x$ ,  $y$ , and  $p_y$  for this situation with  $\sqrt{x}$  and  $\sqrt{y}$  error regions for the position values.

### F. Classical Comparisons

Now, let's say we wished to compare this to a simple, classical system. To do so, we first must get the Hamiltonian from 1, as follows

$$\mathcal{H} = \hbar\omega \left( \frac{p_x^2}{2m_1} + \frac{1}{2}m_1x^2 + \frac{p_y^2}{2m_2} + \lambda e^{x-y} \right)$$

Of course, this is the Hamiltonian of the quantum system, but any quantum method would require the use of the Schrödinger equation to evaluate in a Quantum Mechanical way. Instead, we shall approach this classically using the method of Hamiltonian Mechanics.

Next, we should develop the derivatives of the momenta and spatial variables,

$$\begin{aligned} \dot{x} &= \frac{\partial \mathcal{H}}{\partial p_x} = \hbar\omega \left( \frac{p_x}{m_1} \right) \\ \dot{y} &= \frac{\partial \mathcal{H}}{\partial p_y} = \hbar\omega \left( \frac{p_y}{m_2} \right) \\ \dot{p}_x &= -\frac{\partial \mathcal{H}}{\partial x} = -\hbar\omega (m_1x + \lambda e^{x-y}) \\ \dot{p}_y &= -\frac{\partial \mathcal{H}}{\partial y} = \hbar\omega (\lambda e^{x-y}) \end{aligned}$$



This gives us a set of coupled ODEs, which we can then solve using a relatively simple RK4 method (or RK4(5) if you are so inclined). This shall be done as efficiently as possible using Python.