

# Hamilton-Jacobi Equation and the Semi-classical Approximation

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LIAM FARHAN

*Projektbetreuer:* PROF. DR. PETER BLÖCHL

*Institut für Theoretische Physik*

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# 1 Introduction

The study of molecular dynamics simulations is an essential tool in multiple fields of science such as biophysics [Berendsen 1987], material science [Landman 1988] and drug discovery. It involves modelling the dynamics and interactions of atoms and molecules, which is crucial for developing new materials, understanding protein functions, and designing effective pharmaceuticals. A plethora of methods are employed in this field. Classical Newtonian dynamics [Hug 2013], for example, are effective in simulating large systems but often lack quantum mechanical accuracy. Monte Carlo simulations [Neyts and Bogaerts 2014] provide statistical solutions but can be limited in dynamic representations. On the other hand, ab initio molecular dynamics [Blöchl et al. 2011] have proven more accurate, but at the cost of increased computational demands.

In this project, we investigate a semi-classical approach designed to approximate the solution for the time evolution of the Schrödinger equation:

$$\left[ i\hbar\partial_t - H \left( \frac{\hbar}{i} \vec{\nabla}, \vec{r}, t \right) \right] \psi(\vec{r}, t) = 0, \quad (1)$$

We approach this by employing an Ansatz, expressed as:

$$\psi(\vec{r}, t) = e^{\frac{i}{\hbar} S(\vec{r}, t)}, \quad \text{where} \quad S(\vec{r}, t) = \sum_n \left( \frac{\hbar}{i} \right)^n S_n(\vec{r}, t). \quad (2)$$

Central to our study is the quasi-classical approximation, characterized by  $\hbar \rightarrow 0$ . In this limit, we study the resulting system of equations obtained by expanding eq. (2) up to the first order in  $\frac{\hbar}{i}$ . This expansion yields<sup>1</sup> the following two key equations:

$$\partial_t S_0 + H(\vec{\nabla}_r S_0, \vec{r}) = 0, \quad (3)$$

which is known as the Hamilton-Jacobi equation, and

$$\partial_t S_1 + \frac{\vec{\nabla}_r S_0}{m} \vec{\nabla}_r S_1 + \frac{1}{2m} \vec{\nabla}_r \cdot \vec{\nabla}_r S_0 = 0, \quad (4)$$

which can be related to the real-space particle density  $W(\vec{r}, t)$  using classical trajectories and the continuity equation<sup>2</sup>. As we will later see, eq. (3) offers insights into the phase of the wave function, while eq. (4) relates to its amplitude. Higher order equations in  $\hbar$  can be formulated, providing corrections to these terms, but are not explored in this work. A numerical approach is proposed in [Blöchl 2024] and further detailed in sec. (2.4) to obtain solutions for eq. (3) and eq. (4) from numerical simulations of classical trajectories. This work seeks to formulate this method, further develop it, and test its implementation on concrete physical systems. Among these systems is the quantum harmonic oscillator, whose known quantum solution will be used as a benchmark for this approach in sec. (3.1) and in sec. (3.2). After that, we test this methods on other Hamiltonian systems in sec. (3.3). The results of these tests point at a flaw in this method that is discussed in sec. (4) along with possibilities to resolve this issue.

# 2 Theory

We present in this section the derivation for the equations of motion in sec. (2.1) along with their solution in sec. (2.2) and sec. (2.3). A detailed numerical implementation for the semi-classical method is outlined in sec. (2.4). And the super-position property is discussed in sec. (A).

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<sup>1</sup>For derivation see sec. (2.1)

<sup>2</sup>Blöchl [2024]

## 2.1 Equations of motion in the semi-classical approximation

We start with a general Hamilton operator in the position representation  $H$  with an arbitrary vector potential  $\vec{A}$  and Potential  $V$ . Expanding the Hamiltonian fully yields:

$$H = \frac{1}{2m} \left( \frac{\hbar}{i} \vec{\nabla} - q\vec{A} \right)^2 + V(\vec{r}) = \frac{1}{2m} \left( -\hbar^2 \Delta + q^2 A^2 - q \frac{\hbar}{i} A_i \partial_i - q\hbar \partial_i (A_i) \right) + V(\vec{r}) \quad (5)$$

Our aim is to derive an equation analogous to the time-dependent Schrödinger equation. To this end, we analyze the Hamilton operator's action on the wave function Ansatz  $\psi = e^{\frac{i}{\hbar} S}$ , with  $S$  being a function of position  $\vec{r}$  and time  $t$ . Take the Hamiltonian from eq. (5) and sandwich it between  $e^{\frac{-i}{\hbar} S} H e^{\frac{i}{\hbar} S}$  to obtain:

$$e^{\frac{-i}{\hbar} S} H e^{\frac{i}{\hbar} S} = V(\vec{r}) + \frac{1}{2m} \left( \left( \vec{\nabla}_r S - q\vec{A} \right)^2 + \frac{\hbar}{i} \left( \vec{\nabla}_r^2 S - q\vec{V} \cdot \vec{A} \right) \right)$$

Let's insert this result into the time-dependent Schrödinger equation in the following way:

$$\begin{aligned} (i\hbar\partial_t - H)\psi &= 0 & \text{Ansatz } \psi &= e^{i/\hbar S} \\ (i\hbar\partial_t - H)e^{i/\hbar S} & & \text{multiply from left with } -e^{-i/\hbar S} & \end{aligned}$$

$$\partial_t S + V(\vec{r}) + \frac{1}{2m} \left( \left( \vec{\nabla}_r S - q\vec{A} \right)^2 + \frac{\hbar}{i} \left( \vec{V}_r^2 S - q\vec{V} \cdot \vec{A} \right) \right) = 0 \quad (6)$$

So far we obtained eq. (6), which is the general equation of motion and is equivalent to the Schrödinger equation. Now, we implement semi-classical approximation  $\hbar \rightarrow 0$  to eq. (6). To achieve this, we expand the wave function Ansatz  $\psi = e^{i/\hbar S}$  in terms of  $\frac{\hbar}{i}$ , leading to:

$$S(\vec{r}, t) = \sum_{n=0}^{\infty} \left( \frac{\hbar}{i} \right)^n S_n(\vec{r}, t). \quad (7)$$

We then derive equations for each  $S_n$  from eq. (6) by differentiating eq. (6) with respect to  $\hbar/i$   $n$ -times and subsequently setting  $\hbar \rightarrow 0$ . For convenience we leave out the vector potential  $\vec{A}$  by setting the coupling charge  $q = 0$ . In the zeroth order we obtain an equation for  $S_0$ :

$$\partial_t S_0 + V(\vec{r}) + \frac{1}{2m} \left( \vec{\nabla}_r S_0 \right)^2 = 0, \quad (8)$$

which is the well known Hamilton-Jacobi equation. In the first order, we derive the equation of motion by applying  $\partial_{\frac{\hbar}{i}}$  to eq. (6), setting  $q = 0$  and  $\hbar \rightarrow 0$ , resulting in the equation for  $S_1$ :

$$\partial_t S_1(\vec{r}, t) + \frac{1}{m} \vec{\nabla}_r S_0(\vec{r}, t) \vec{\nabla}_r S_1(\vec{r}, t) + \frac{1}{2m} \vec{\nabla}_r \vec{\nabla}_r S_0(\vec{r}, t) = 0 \quad (9)$$

Using the semi-classical approximation, we reduced the time-dependent Schrödinger equation to a system of coupled partial differential equations for  $S_0$  in eq. (3) and  $S_1$  eq. (4). The solution for this system  $\psi(\vec{r}, t)$  must satisfy the boundary conditions for a wave function defined at an initial time point  $\psi(\vec{r}, t = 0)$ . From the real part we get  $S_1(\vec{r}, t = 0) = \text{Re log } \psi(\vec{r}, 0)$ , while the imaginary part gives us the relations  $S_0(\vec{r}, t = 0) = \hbar \text{Im log } \psi(\vec{r}, 0)$  and  $\vec{\nabla}_r S_0(\vec{r}, t = 0) = \hbar \vec{\nabla}_r \text{Im log } \psi(\vec{r}, 0)$

## 2.2 Solution of $S_0$ from classical trajectories

In his work, Blöchl [2024] proposes solving this system of partial differential equations along trajectories  $\gamma(t) = (\vec{R}(t), \vec{P}(t))$  rather than solving it globally. In this section we outline this method for  $S_0$ . First, we assume  $S_0$  is defined along the trajectory such that  $S_0(\vec{R}(t), t)$  is given. Second, we define the variable  $\vec{P}(t)$  as the gradient of

$S_0$  along the trajectory:  $\vec{P}(t) = \vec{\nabla}_r S_0(\vec{R}(t), t)$ . Taking the total derivative with respect to  $t$  of eq. (3) yields:

$$\frac{d}{dt} S_0(\vec{R}(t), t) = \underbrace{\partial_t S_0(\vec{R}(t), t)}_{-H(\vec{P}, \vec{R})} + \underbrace{\vec{\nabla}_r S_0(\vec{R}(t), t)}_{\vec{P}(t)} \cdot \dot{\vec{R}}(t), \quad (10)$$

which cannot be integrated unless  $\vec{P}(t)$  is known. To determine it, we take the total time derivative and obtain:

$$\frac{d}{dt} \vec{P}(t) = -\vec{\nabla}_r H(\vec{P}(t), \vec{R}(t)) + \left( \dot{\vec{R}}(t) - \vec{\nabla}_p H(\vec{P}(t), \vec{R}(t)) \right) \vec{\nabla}_r \otimes \vec{\nabla}_r S_0(\vec{R}(t), t). \quad (11)$$

This, also cannot be solved easily due to the term containing  $\vec{\nabla}_r \otimes \vec{\nabla}_r S_0(\vec{R}(t), t)$ , which requires prior knowledge of  $S_0$  both in the tangential and perpendicular directions of  $\vec{R}$ . To overcome this difficulty, Blöchl [2024] proposes adding a constraint on the trajectory such that this cumbersome term vanishes. This is achieved by selecting a trajectory that makes the factor in parentheses vanish, coinciding with the classical trajectories obeying Hamilton's equations:

$$\dot{\vec{R}} = \vec{\nabla}_P H(\vec{P}, \vec{R}, t) \quad \& \quad \dot{\vec{P}} = -\nabla_r H(\vec{P}, \vec{R}, t) \quad (12)$$

Along such trajectories  $S_0$  simply becomes the classical action:

$$S_0(\vec{R}(t), t) = S_0(\vec{R}(0), 0) + \int_{[\vec{P}, \vec{R}]} dt' \left( -H(\vec{P}(t'), \vec{R}(t')) + \vec{P}(t') \cdot \vec{R}(t') \right) \quad (13)$$

### 2.3 Solution for $S_1$ from the particle density

By employing the same choice of trajectories and utilizing the particle conservation law, a solution for  $S_1$  in eq. (4) can be derived from the real-space particle density distribution  $W(\vec{r}, t)$ :

$$S_1(\vec{R}(t), t) = S_1(\vec{R}(0), 0) + \frac{1}{2} \log \frac{W(\vec{R}(t), t)}{W(\vec{R}(0), 0)}. \quad (14)$$

While the selection of  $W(\vec{R}(0), 0)$  is arbitrary, a logical and natural choice would be to set  $W(\vec{r}, t) = |\psi(\vec{r}, t)|^2$ . Let us denote  $\gamma := (\vec{r}, \vec{p}, t_0)$  as a set of coordinates that uniquely identify a particle trajectory within a classical Hamiltonian system. These are meant to be read as: the trajectory crosses the point  $\vec{r}$  with momentum  $\vec{p}$  at time  $t_0$ . Thus, a trajectory  $\vec{R}_i$  that crosses  $\gamma_i$ , i.e.  $\vec{R}_i(t_0, \gamma) = \vec{r}$  is unique due to the Liouville theorem. With this notation, we give an analytical solution for the particle density. To this end, we work in phase space, as it enables the use of the Liouville theorem. Start by promoting the particle density  $W(\vec{r}, t)$  to the phase-space density function  $\rho(\vec{r}, \vec{p}, t)$ . The phase-space density has the following properties:

- At the initial time  $t = 0$ , its value is given by

$$\rho(\vec{r}, \vec{p}, 0) = W(\vec{r}, 0) \delta(\vec{p} - \vec{\nabla} S_0(\vec{r}, t=0)), \quad (15)$$

- It evolves in time according to the Liouville equation, where  $\{.,.\}$  denotes the Poisson brackets:

$$\frac{d}{dt} \rho(\vec{r}, \vec{p}, t) = \{H(\vec{p}, \vec{r}, t), \rho(\vec{r}, \vec{p}, t)\} \quad (16)$$

- The particle density  $W(\vec{r}, t)$  is obtained from  $\rho$  by marginalizing over the momentum:

$$W(\vec{r}, t) = \int \rho(\vec{r}, \vec{p}, t) d^3 p. \quad (17)$$

Solving the Liouville equation can be done with the method of characteristics<sup>3</sup> which states that  $\rho(\vec{r}, \vec{p}, t)$  is constant along classical trajectories, i.e.  $\rho(\vec{R}(t_1, \gamma), \vec{P}(t_1, \gamma), t_1) = \rho(\vec{R}(t_2, \gamma), \vec{P}(t_2, \gamma), t_2)$  for arbitrary  $t_1$  and  $t_2$  and fixed  $\gamma$ . Thus, the particle density is obtained with:

$$\rho(\vec{R}(t), \vec{P}(t), t) = W(\vec{R}(0), 0) \delta(\vec{P}(0) - \vec{\nabla}_r S_0(\vec{r}, t=0)) \quad (18)$$

$$\Rightarrow W(\vec{R}(t), t) = \sum_{\vec{p}_i} W(\vec{R}(0, \gamma_i), 0) \left| \frac{1}{\frac{\partial}{\partial p_i} \vec{P}(0, \gamma_i)} \right|. \quad (19)$$

Here  $\gamma_i$  are defined to cross the trajectory in position space at time  $t$  and cross the trajectory in momentum space at the initial time.  $\gamma_i = (\vec{R}(t), \vec{p}_i, t)$  and  $\gamma_i = (\vec{R}(0), \vec{\nabla}_r S_0(\vec{R}(0), 0), 0)$ . In many systems, multiple trajectories meet these criteria, resulting in the summation in eq. (18) due to the characteristics of the delta function<sup>4</sup>

## 2.4 Numerical implementation

To realize the solution for eq. (3) and eq. (4) numerically Blöchl [2024] outlines the following numerical approach:

- Begin with  $N$  particles distributed according to the initial wave function  $W(\vec{r}, t=0) = |\psi(\vec{r}, t=0)|^2$ .
- Assign for each particle at position  $\vec{r}$  an initial momentum  $\vec{p}(r, t=0) = \vec{\nabla}_r \arg \psi(\vec{r}, t=0) = \vec{\nabla}_r S_0(\vec{r}, 0)$ .
- Evolve the particles using classical equations of motion eq.(12) and simultaneously, integrate the classical action along their trajectories to find the zeroth-order action  $S_0(\vec{r}, t)$ .
- Compute the particle density  $W(\vec{r}, t)$  at time  $t$  and obtain the first-order action  $S_1(\vec{r}, t)$  from this density.
- Formulate the wave function using both actions:

$$\psi(\vec{R}(t), t) = \sqrt{W(\vec{R}(t), t)} \exp \left\{ \left( \frac{i}{\hbar} S_0(\vec{R}(t), t) + i \arg \{ \psi(\vec{R}(0), 0) \} \right) \right\} \quad (20)$$

In this project, we employ the velocity Verlet method for trajectory integration, which involves the following steps:

$$\vec{R}(t+dt) = \vec{R}(t) + \frac{1}{m} \vec{P}(t) dt + \frac{1}{2} \vec{a} dt^2 \quad (21)$$

$$\frac{1}{m} \vec{P}(t+dt) = \frac{1}{m} \vec{P}(t) + \frac{1}{2} (\vec{a}(t+dt) + \vec{a}(t)) dt \quad (22)$$

$$S_0(\vec{R}(t+dt)) = S_0(\vec{R}(t)) + \frac{1}{m} \vec{P}^2(t) - H(\vec{P}(t), \vec{R}(t), t), \quad (23)$$

with  $\vec{a}(t) = \dot{\vec{P}} = -\nabla_r H(\vec{P}, \vec{R}, t)$  and  $\frac{1}{m} \vec{P}(t) = \dot{\vec{R}}(t)$ . For initializing the particles with a certain position probability distribution  $W(\vec{R}(0), 0)$ , we employ the von neumann sampling method. This involves the following steps:

- Generate a random position  $\vec{R}$  from the desired spatial domain and a test number  $y$  from a uniform distribution in the range  $[0, 1]$ .
- Check the acceptance criterion  $y \leq W(\vec{R}, 0)$ . This step determines whether the randomly chosen position  $\vec{R}$  is consistent with the probability distribution  $W$ .
- If the criterion is not met, reject the sampled position  $\vec{R}$  and return to the first step for a new sample.
- If the criterion is full filled, place a particle at position  $\vec{R}$  with momentum  $\vec{P} = \vec{\nabla}_r S_0(\vec{R}, 0)$ .

<sup>3</sup>A short proof for this is sketched in the appendix.

<sup>4</sup> $\delta(f(p)) = \sum_{h_i} \frac{1}{|f'(p)|} \delta(p - h_i)$  where  $h_i$  are zeros of  $f$

By initiating the particles with a specific density  $W(\vec{R}, 0)$  and evolving their trajectories numerically with the velocity Verlet method, obtaining the density becomes a simple measurement: To determine the particle density at a given time  $t$  and position  $\vec{r}$ , we consider a small interval centered at  $\vec{r}$  with width  $dr$ , denoted as  $[r - dr, r + dr]$ . Within this interval, we count the number of particles  $N[r - dr, r + dr]$  that landed there. The particle density  $W(\vec{r}, t)$  is estimated by the proportion  $\frac{N[r - dr, r + dr]}{N}$ , where  $N$  is the total number of particles in the system.

### 3 Results and discussion

Having outlined the semi-classical method, we now test said method on concrete quantum systems.

#### 3.1 One-Dimensional Harmonic Oscillator

Let's consider a simple one-dimensional harmonic oscillator with the Hamilton operator:

$$\hat{H} = \frac{\hat{P}^2}{2m} + \frac{1}{2}m\omega^2\hat{X}^2 \quad (24)$$

The oscillator starts in an initial state described by the wave function:

$$\psi(\vec{x}, t = 0) = \sqrt{\frac{\lambda}{\sqrt{\pi/2}}} e^{-\lambda^2(\vec{x} - \vec{\mu})^2} e^{i\frac{\vec{p}_0 \cdot \vec{x}}{\hbar}}. \quad (25)$$

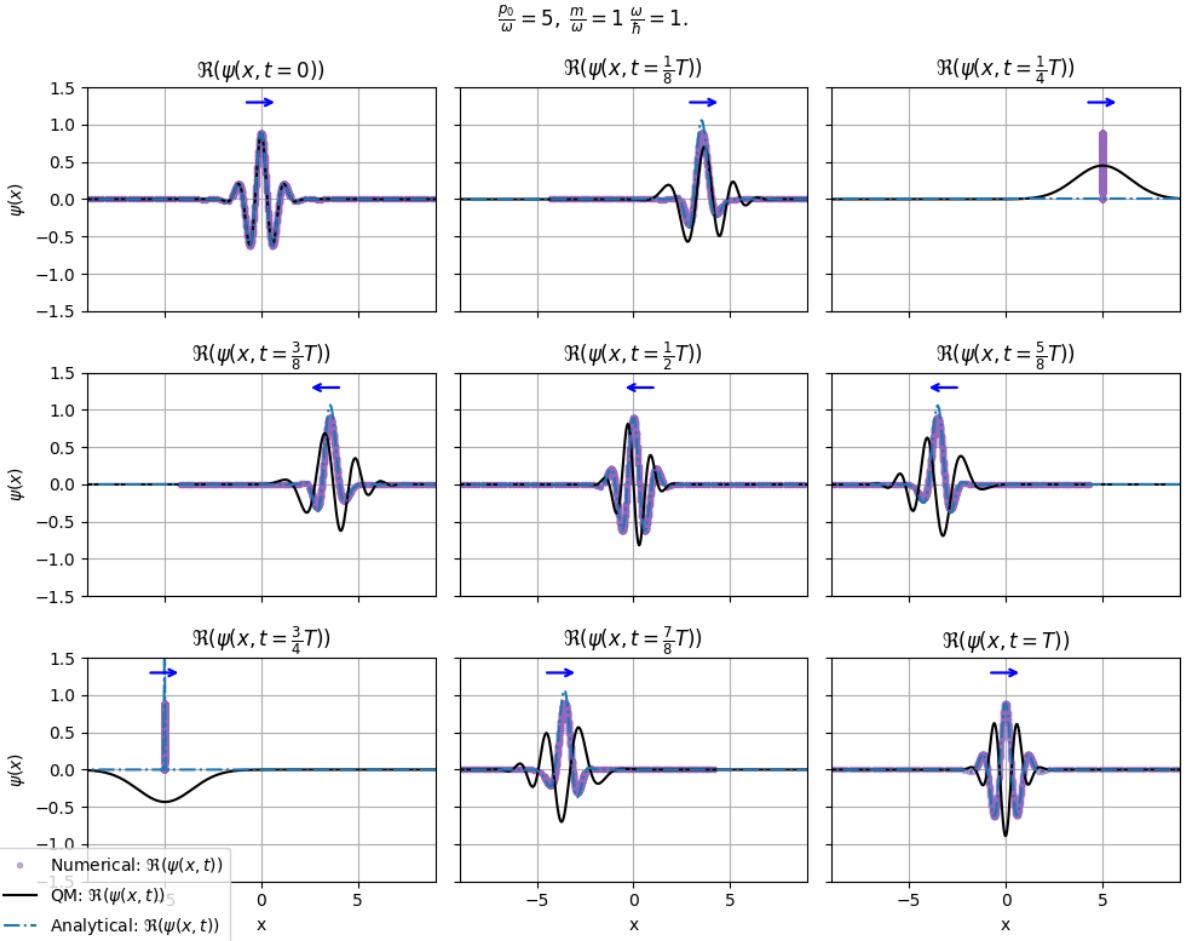
The system is simple enough, that a direct analytical solution for the semi-classical equations (3) and (4) is possible. A derivation for this solution is presented in the appendix, and it will be used as a baseline of comparison to test the semi-classical method. In this section we compare both the numerical implementation and the analytical solution of the semi-classical method with the pure quantum time evolution of the system<sup>5</sup>. Note that the quantum time-evolution involves evaluating an infinite summation series, which, for numerical implementation, must be truncated after a finite number of terms. This truncation is justified by the fact that including more terms yields diminishing returns, in proportion to  $\frac{1}{\sqrt{2^n n!}}$ . The value of the truncation is determined at the point where the large numbers involved cause an overflow error. Note that additional terms at this point do not contribute to any visible difference in the wave function. A set of parameters in the semi-classical regime  $p_0 = 5\frac{\hbar}{\omega}$  is chosen for our comparison. In Figure (1), we present the real part of the time-evolved wave function using both methods at various time points, and make the following observations:

- For the semi-classical method, there is an exact agreement between the numerical implementation and the analytical solution.
- The form of the wave function as predicted by the numerical method closely aligns with that of the quantum time evolution. The overall shapes and periodic motion of the wave functions are in agreement.
- Nonetheless, a noticeable discrepancy is observed at the inflection points. While the semi-classically time-evolved wave function collapses into a single delta-like peak at the classical turning points, the quantum time-evolved wave function does not and gets reflected at slightly delayed turning points by comparison. As a result of this delay, a noticeable phase shift emerges following each turning point between the two solutions. Specifically, the quantum time-evolved solution leads with a phase difference of  $\frac{\pi}{2}\hbar\omega$ .
- Furthermore, the phase difference accumulates after each turn, causing both solutions to have opposite phases after one period and then return to matching phases after two complete periods.

The overall agreement between the semi-classical and quantum solutions, as shown in Figure (1), indicates that the discussed semi-classical method is capable of capturing the main features of the Schrödinger equation in the

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<sup>5</sup>See appendix for derivation



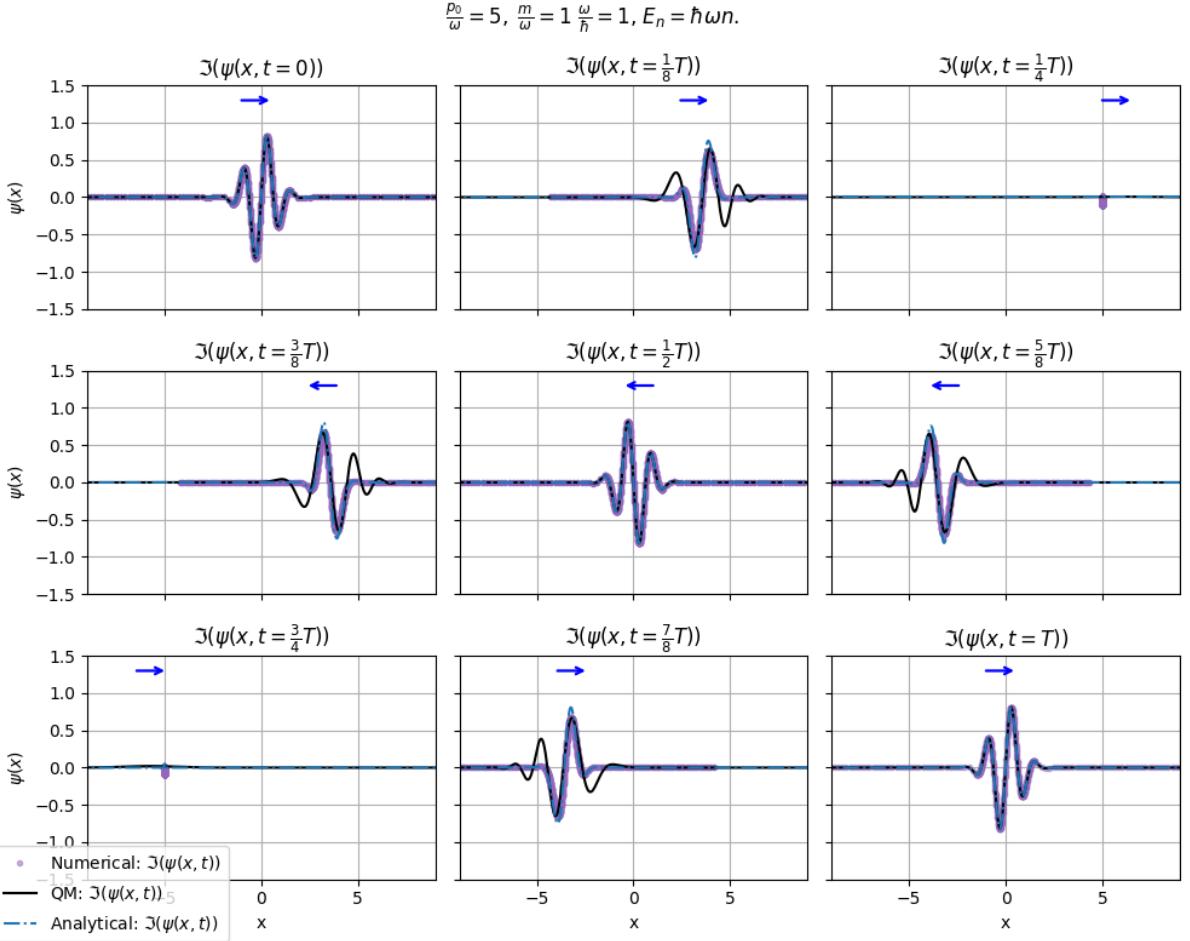
**Figure 1:** Time Evolution of the Wave Function for a One-Dimensional Harmonic Oscillator. This plot illustrates the real part of the wave function with the initial value from eq. (25), as it evolves over time. The harmonic oscillator is described by the Hamiltonian in eq. (24) and the evolution is analyzed using both numerical (2.4) and analytical<sup>6</sup> methods, which are then compared to the quantum time evolution<sup>7</sup>. The parameters:  $\frac{p_0}{\omega} = 5, \frac{m}{\omega} = 1, \frac{\omega}{\hbar} = 1$  are chosen for this comparison. The blue arrow indicates the direction of propagation of the wave function.

case of the harmonic oscillator. The collapse of the semi-classical solution at the turning points into a delta peak is reflected in the the analytical solution<sup>8</sup> and it appears to be a specific feature of this system<sup>9</sup>. However, the apparent phase shift between the two methods needs to be explained. A key observation for this is the later inflection point in the quantum time-evolution, suggesting the presence of higher energy compared to the semi-classical method. It is a well-established fact that quantum harmonic oscillators possess zero point energies, which is not the case for classical oscillators. To investigate whether this zero point energy contributes to the observed difference, we change the quantum solution by artificially removing the zero point energy, setting  $E_n = \hbar\omega n$  instead of  $E_n = \hbar\omega(n + \frac{1}{2})$ <sup>10</sup>. With this modification, we recompute the solution for the quantum time evolution and compare the results with the semi-classical method in Figure (2). It's important to note that, for this comparison, we chose to examine the imaginary part of the wave function. This serves as a consistency check, since the imaginary part should exhibit a simple phase shift relative to the real part. The behavior of the wave function remains consistent across both its real and imaginary components, regardless of the part being analyzed. We observe in Figure (2) that the quantum and semi-classical solutions align with the removal of the zero point energy of the quantum oscillator. This adjustment effectively eliminates the phase shift that was previously observed following the inflection points. As previously mentioned, the imaginary part of the wave function exhibits a phase shift relative to the real part.

<sup>8</sup>See App.

<sup>9</sup>Later systems do not exhibit such behaviour.

<sup>10</sup>This is also equivalent to adding the zero point energy to the semi-classical method.



**Figure 2:** Comparison of Quantum and Semi-Classical Solutions after Removing the Zero Point Energy. The exact set up as detailed in Figure 1 is used for the computation, but with a key modification in the quantum time evolution: the energy levels are set to  $E_n = \hbar\omega n$  instead of  $E_n = \hbar\omega(n + \frac{1}{2})$ .

This observation is in agreement with expectations and serves as an indicator of the correct implementation of the methods. While the observed phase shift can be attributed to the zero-point energy of the harmonic oscillator, it's important to consider that other factors might also play a role. In particular, the analytical solution of the semi-classical method exhibits discontinuities at the classical turning points. This raises the possibility that selecting a different branch of the logarithm, and consequently introducing a phase shift of at each turning point could be necessary to achieve continuity. Nevertheless, as of now, there is no formal justification for this approach and it should be considered for further analysis.

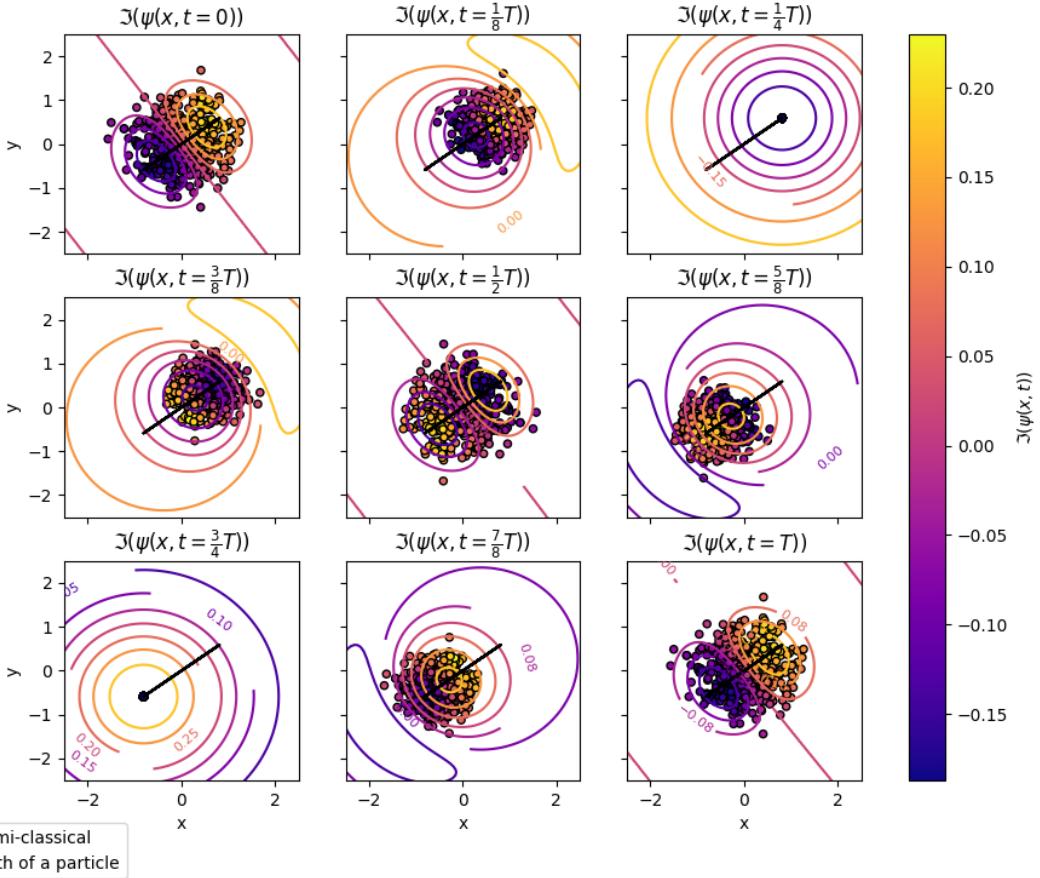
### 3.2 Two-Dimensional Harmonic Oscillator

We now focus on Harmonic oscillator in 2D. This serves as a test, as the semi-classical method is intended for higher dimensional systems. Similar to the previous section, obtaining the solution for the quantum time evolution is straightforward. We evolve an initial wave function within a Hamiltonian system, expressed as:

$$\psi(\vec{r}, t = 0) = \frac{\lambda}{\sqrt{\pi/2}} e^{-\lambda^2(\vec{r}-\vec{\mu})^2} e^{i\frac{\vec{p}_0 \cdot \vec{r}}{\hbar}}, \quad \hat{H} = \frac{1}{2m} \hat{P}^2 + \frac{1}{2} m \hat{X}^2 \omega_1^2 + \frac{1}{2} m \hat{Y}^2 \omega_2^2. \quad (26)$$

First, we observe the motion, with an initial momentum in a set direction  $\vec{p}_0 = \begin{pmatrix} \cos \frac{\pi}{5} \\ \sin \frac{\pi}{5} \end{pmatrix}$ . This is done without removing the zero-point energy in the quantum time evolution. The results are shown in fig. 3. Similar to the

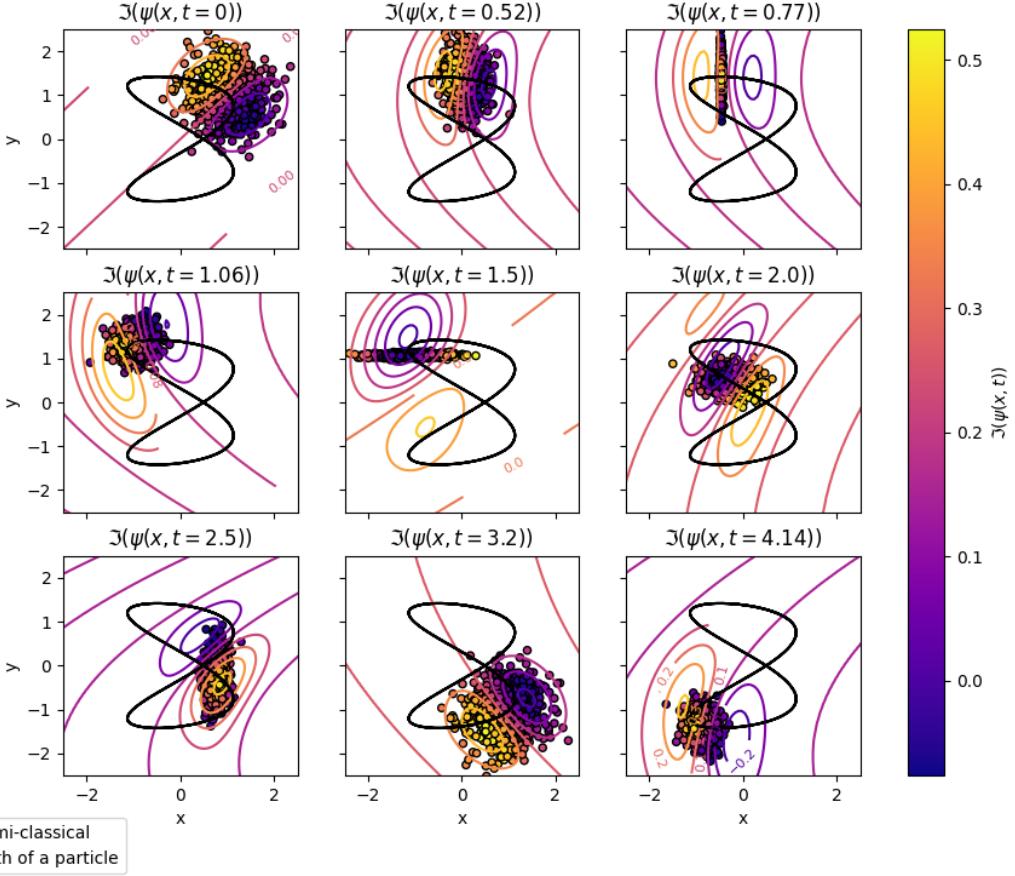
$$\frac{\vec{p}_0}{\omega_1} = (\cos \frac{\pi}{5}, \sin \frac{\pi}{5}), \frac{m}{\omega_1} = 1, \frac{\omega_1}{\hbar} = 1, \frac{\omega_2}{\hbar} = 1, E_{n,m} = \hbar\omega_1(n + \frac{1}{2}) + \hbar\omega_2(m + \frac{1}{2}).$$



**Figure 3:** Time Evolution of the 2D Harmonic Oscillator. Two methods are compared: the semi-classical method outlined in sec. [2.4] and the quantum time evolution method. The particles represent the semi-classical method, while the contour plot shows the quantum time evolution. The black line traces the classical motion of the centre point of the wave function. We view the wave function at multiple time points. Zero point energy is present, the motion starts in a line.

one-dimensional case, there is a phase offset that becomes apparent after the first turning point. Moreover, the semi-classically evolved wave function collapses into a delta peak at that point. Note that removing the zero point energy from the quantum time evolution indeed eliminates the mentioned phase shift. This plot does not reveal extraordinary information, because the oscillator is moving in a linear motion without any angular component. This motion can be simplified to a one-dimensional oscillator, by implementing a coordinate rotation setting the axis of motion to the x-direction. A much more interesting comparison is presented in fig. [4]. There the centre  $\vec{\mu}$  of the wave function is offset from the origin, and the initial momentum  $\vec{p}_0$  is set in the tangential direction of the centre, i.e.  $\vec{p}_0 = |\vec{\mu}| \hat{e}_\theta$ , with  $\hat{e}_\theta = \begin{pmatrix} \cos \theta \\ -\sin \theta \end{pmatrix}$ ,  $\theta = \arctan \frac{\mu_y}{\mu_x}$ . This insures a rotational motion around the origin. Next, the oscillator frequencies are chosen as  $\omega_1 = 1$ ,  $\omega_2 = 2$ , to investigate the effect of non-equal frequencies. The quantum time evolution is done with the zero points energy removed. We observe in fig. [4] an overall agreement between the two methods, both in the motion trajectory and the phase. An interesting effect emerges due to the different frequencies: The semi-classical method wave function collapse occurs for each direction of motion independent of the other. For instance we notice at  $T = 0.77$  the collapse is in the x direction and at  $T = 1.5$  the collapse in the y-direction. Due to the different frequencies, the overall trajectory follows a self-intersecting curve. Despite the complicated path of the oscillator, the semi-classical method is capable of replicating the harmonic oscillator motion successfully. It, however, fails to account for the zero point energy of the quantum system as discussed earlier.

$$\frac{\tilde{p}_0}{\omega_1} = |\vec{p}| \hat{e}_\theta, \frac{m}{\omega_1} = 1, \frac{\omega_1}{\hbar} = 1, \frac{\omega_2}{\hbar} = 2, E_{n,m} = \hbar\omega_1 n + \hbar\omega_2 m.$$



**Figure 4:** Time Evolution of the 2D Harmonic Oscillator. Two methods are compared: the semi-classical method outlined in sec. [2.4] and the quantum time evolution method. The particles represent the semi-classical method, while the contour plot shows the quantum time evolution. The black line traces the classical motion of the centre point of the wave function. We view the wave function at multiple time points. Zero point energy is removed, the motion starts in the tangential direction of the centre point of the wave function.

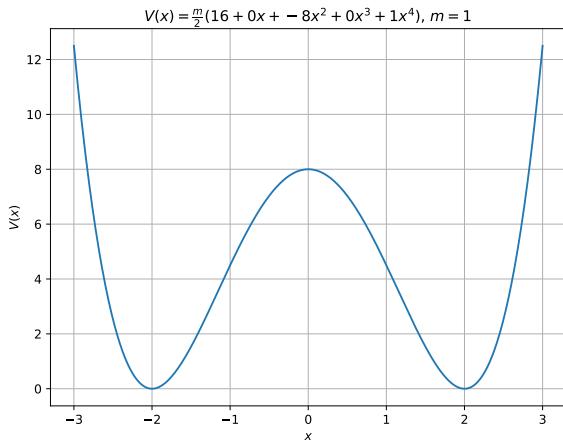
### 3.3 Other Hamiltonian systems

This section concerns exploring more complicated Hamiltonian systems. We consider the following Hamilton operator:

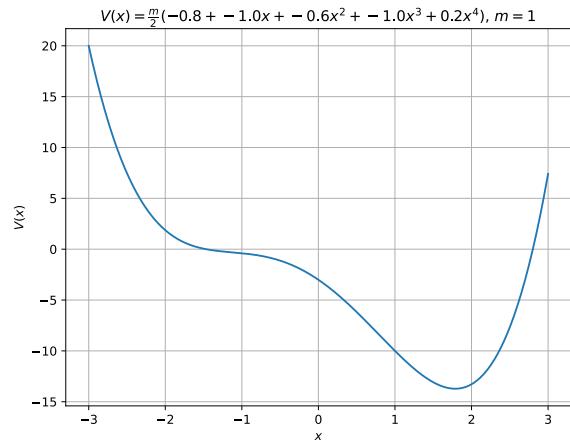
$$\hat{H} = \frac{1}{2m} \hat{P}^2 + \frac{m}{2} \left( a_0 + a_1 \hat{X} + a_2 \hat{X}^2 + a_3 \hat{X}^3 + a_4 \hat{X}^4 \right), \quad (27)$$

with a various set of parameters  $\{a_i\}$  and normalized units such that mass  $m = 1$  and  $\hbar = 1$ . In fig. (5) the potential for two such parameter sets is shown. We evolve the initial conditions given in eq. (25) using the semi-classical method explained in sec. (2.4). Starting with a symmetric potential (fig. (5a)) and an initial momentum  $p_0 = 1$ , we obtain the result shown in fig. (6). Note that, no quantum time evolution is shown for comparison.

This system presents an apparent flaw in the semi-classical method under consideration. The wave function appears to be multi valued, which is problematic since that cannot be a function. This behavior arises from the employed numerical method that simulates multiple particles. Initially, certain particles move in the positive x-direction, while others descend with the potential in the negative x-direction, as observed at  $t = 0.78$  in fig. (3). At a later time,  $t = 1.57$  both waves get reflected and overlap the incoming waves. The numerical method doesn't have a logic to handle multiple particles present at the same location with different action  $S_0$  values. Due to this multiple solutions are present at the same coordinates  $(x, t)$ . With each new reflection, more solutions overlap, e.g. at  $t = 3.92$ . This is illustrated more clearly in fig. (7), that shows the time evolution with the potential shown in fig. (5b). The potential is asymmetric, which causes the wave function to be concentrated in the low potential

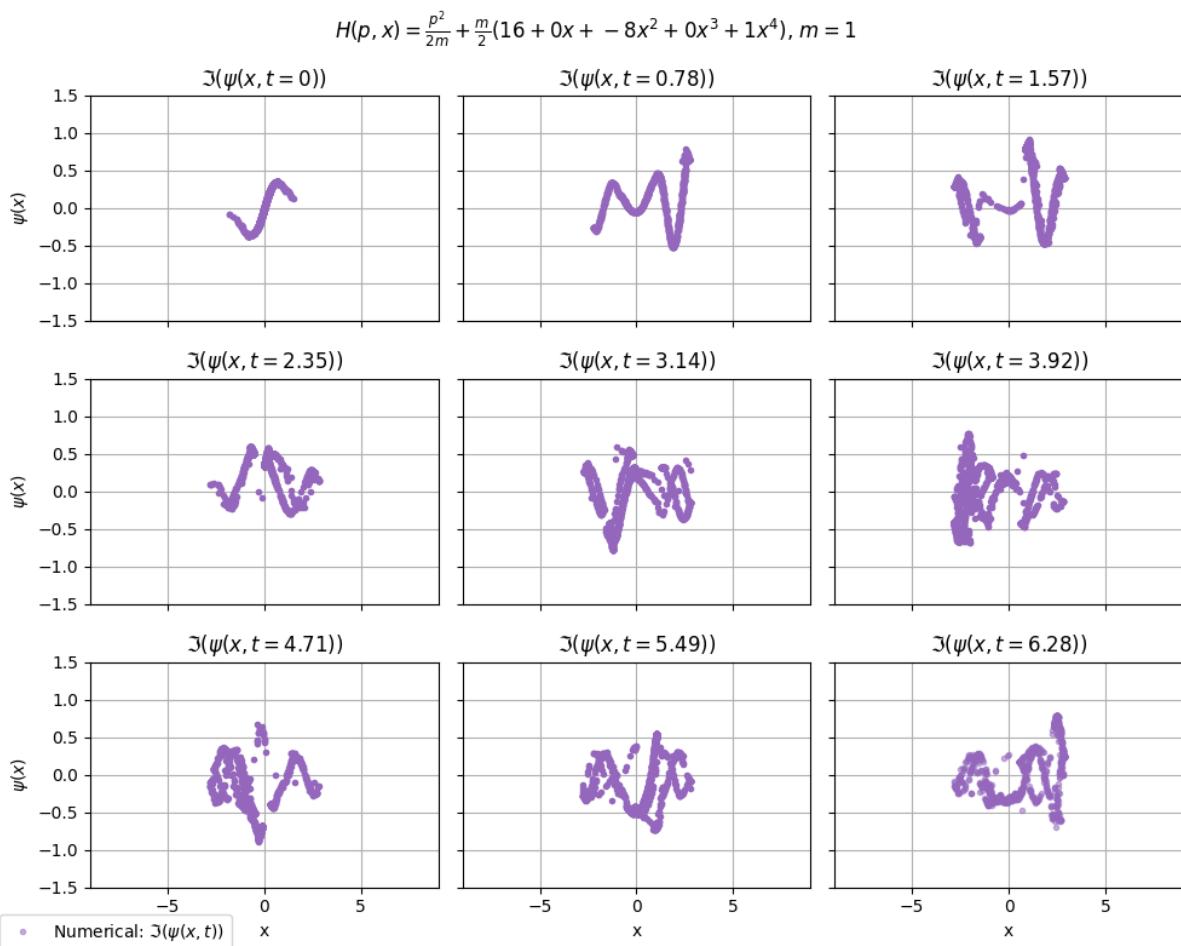


**(a) Symmetric potential**



**(b)** Deeper potential well on the right

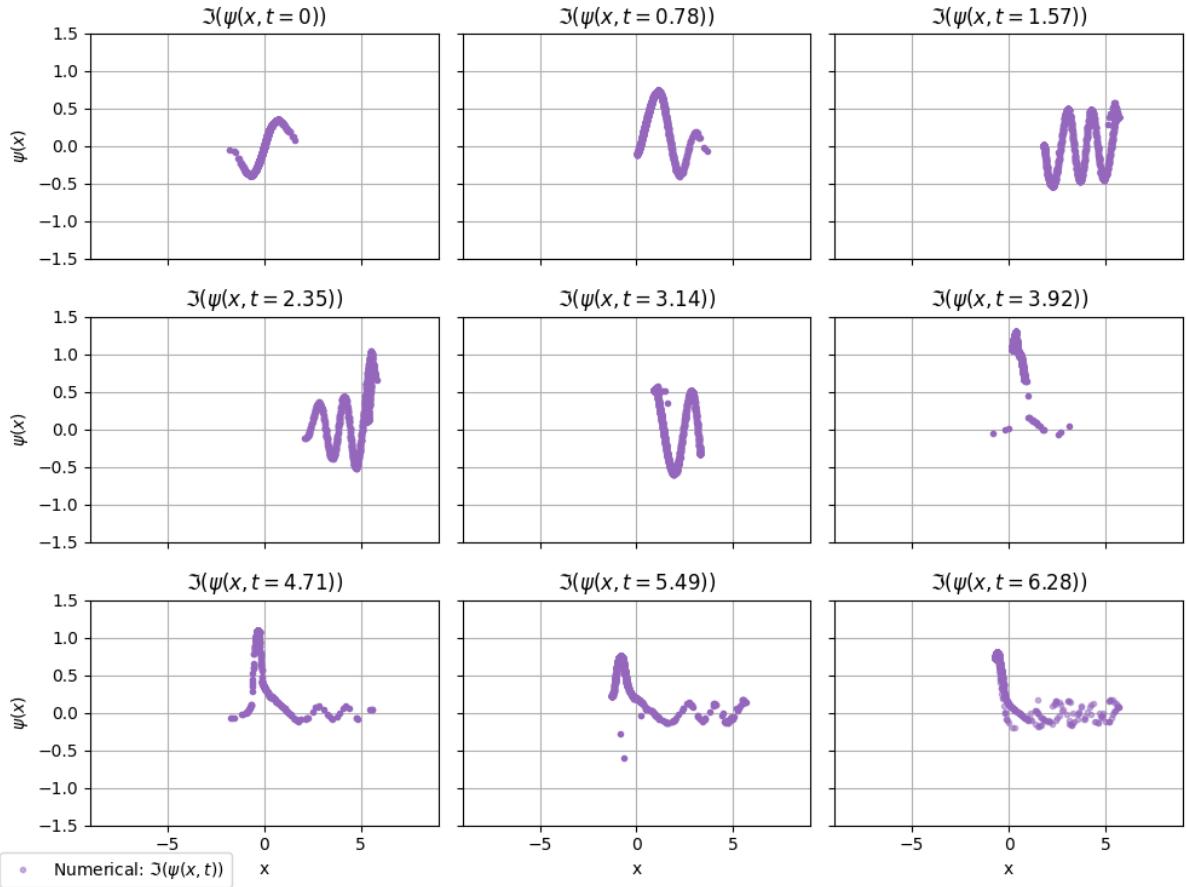
**Figure 5:** Potential of the Hamilton system from eq. (27) with different parameter values.



**Figure 6:** Semi-classical time evolution of the wave function from eq. (25) in the Hamilton system from eq. (27) and the symmetric potential shown in fig. (5a) presented at multiple time points.

region. At  $t = 5.49$  and  $t = 6.28$  we can see the incoming and reflected waves overlapping clearly.

$$H(p, x) = \frac{p^2}{2m} + \frac{m}{2}(-0.8 + -1.0x + -0.6x^2 + -1.0x^3 + 0.2x^4), m = 1$$



**Figure 7:** Semi-classical time evolution of the wave function from eq. (25) in the Hamilton system from eq. (27) and the assymetric potential shown in fig. (5b) presented at multiple time points.

## 4 Discussion and outlook

In this work we investigated the semi-classical method outlined in sec. (2.1) and its numerical implementation described in sec. (2.4). Testing the method on the Harmonic oscillator revealed an agreement with the quantum time evolution. The semi-classical method is capable of producing the predicted wave form and behaviour. It, however, differs from the quantum time evolution in multiple ways. Firstly, at the classical turning points, the wave form collapses into a delta like peak. This behavior is explained by the density term or  $S_1$  and is unique for the harmonic oscillator. Particles starting at a Gaussian distribution and a constant momentum reach the classical turning point at the same time in a Hamiltonian system with a harmonic potential. Secondly, the semi-classical method in its current implementation fails to account for the zero point energy of the quantum harmonic oscillator. This manifests as a phase difference  $\frac{\pi}{2}\hbar\omega$  that occurs after each turning point between the two methods. Adjusting for this artificially by setting  $E_n = \hbar\omega n$  instead of  $E_n = \hbar\omega(n + \frac{1}{2})$  accounts for the phase difference, which indicates that  $S_0$  is missing an additional term  $\frac{\hbar\omega}{2}$ . Nothing in eq. (13) indicates such term. Moreover, choosing a different branch for  $S_0$  does not account for this phase difference either, since a different branch will contribute a phase of  $2\pi k$ . Arguments of continuity at the classical turning points may lead to a phase increase. Nevertheless, this is unlikely, as the phase difference is persists during the entire motion and not just at the turning points. It's most apparent there due to the wave collapse. More analysis in this area is needed in general. With the zero point energy accounted for, the semi-classical method is capable of precisely predicting the motion of the 2D harmonic oscillator as can be seen in fig. (4).

Investigating other Hamiltonian systems revealed an issue with the semi-classical method discussed in this

work. For the asymmetric and the symmetric potentials shown in fig. (5) the numerical simulation yields multiple solutions for the wave function for identical coordinates  $(t,x)$ . This behaviour excludes the solution from being a mathematical function. To understand this issue we turn to the terms of the solution used in the semi-classical method eq. (20). Given that  $W$  is uniquely defined at each point of space as the particle density, cannot be responsible for the observed behavior. This singles out  $S_0$  as the culprit: The way  $S_0$  is computed at the position  $\vec{R}(t)$  and time point  $t$  is related to the value of  $S_0$  at  $\vec{R}(0)$  and the initial time point  $t = 0$ . This implicitly assumes a unique solution for the trajectory, i.e. there exists only one trajectory and only one initial coordinate  $\vec{R}(0) \gamma$ , such that for  $t$ :  $\gamma = (\vec{R}(t), \vec{P}(t), t)$  and for  $t = 0$ :  $\gamma = (\vec{R}(0), \vec{\nabla}_r S_0(\vec{R}(0)), 0)$ . This is a necessary condition for  $S_0$  as defined in eq. (13) to have a unique solution. While the Liouville theorem states that trajectories in phase space don't intersect, we note that this system is under determined: multiple trajectories  $\gamma_i$  can cross  $\vec{R}(t)$  albeit with differing momenta  $\vec{P}_i(t)$  and differing initial coordinates  $\gamma_i = (\vec{R}_i(0), \vec{\nabla}_r S_0(\vec{R}_i(0)), 0)$ . The numerical simulation of the particles reveals this as the multiple solutions for the wave function in the Hamiltonian system from sec. (3.3).

We suggest investigating the solution of the Hamilton-Jacobi to resolve this issue. A commonly used method for solving the Hamilton-Jacobi equation is the so called Hopf-Lax formula [Chow et al. 2017] suggests taking the initial coordinate with the minimal action  $S_0$  as the solution.

$$\varphi(x, t) = \min_{v \in R^d} \left\{ g(\gamma(v, 0)) + \int_0^t \{ \langle p(v, s), \partial_p H(\gamma(v, s), p(v, s), s) \rangle - H(\gamma(v, s), p(v, s), s) \} ds \right\}, \quad (28)$$

with

$$\dot{\gamma}(v, s) = \partial_p H(\gamma(v, s), p(v, s), s), \quad (29)$$

$$\dot{p}(v, s) = -\partial_x H(\gamma(v, s), p(v, s), s), \quad \gamma(v, t) = x, p(v, t) = v. \quad (30)$$

This is an active area of research, as the Hamilton-Jacobi equation plays an important role in viscosity calculations [Barles 2013], quantum gravity [Kiefer 1994] and control theory [Misztela 2020].

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## A Super position principle

If we wish to model the time evolution of a superposition of Wave functions  $\psi_1(\vec{r}, t = 0) = \sqrt{W_1(\vec{r}, 0)}e^{\frac{i}{\hbar}S_0^1(\vec{r})}$  and  $\psi_2(\vec{r}, t = 0) = \sqrt{W_2(\vec{r}, 0)}e^{\frac{i}{\hbar}S_0^2(\vec{r})}$ , the result is not a straightforward superposition of the time-evolved wave functions  $\psi(\vec{r}, t) \neq \psi_1(\vec{r}, t) + \psi_2(\vec{r}, t)$ . This is a direct consequence of the fact that the equations governing the time evolution of  $S_0$  and  $S_1$  are not linear. In this section we present a way to sum two wave functions in the semi-classical approximation. To begin set  $\psi(\vec{r}, t = 0) = \psi_1(\vec{r}, 0) + \psi_2(\vec{r}, 0) =: \sqrt{W(\vec{r}, 0)}e^{\frac{i}{\hbar}S_0(\vec{r}, 0)}$ . We note that any wave function the density is given by  $W(\vec{r}, t = 0) = |\psi(\vec{r}, 0)|^2$  and the initial phase is given by  $S_0(\vec{r}, 0) = \hbar \arg \psi(\vec{r}, 0)$ . Thus we can employ simple complex number arithmetic to arrive at the relations:

$$W(\vec{r}, t = 0) = W_1(\vec{r}, 0) + W_2(\vec{r}, 0) + 2\sqrt{W_1(\vec{r}, 0)W_2(\vec{r}, 0)} \cos\left(\frac{1}{\hbar}S_0^1(\vec{r}, 0) - \frac{1}{\hbar}S_0^2(\vec{r}, 0)\right) \quad (31)$$

$$S_0(\vec{r}, t = 0) = \hbar \arctan\left(\frac{\sqrt{W_1(\vec{r}, 0)} \sin\left(\frac{S_0^1(\vec{r}, 0)}{\hbar}\right) + \sqrt{W_2(\vec{r}, 0)} \sin\left(\frac{S_0^2(\vec{r}, 0)}{\hbar}\right)}{\sqrt{W_1(\vec{r}, 0)} \cos\left(\frac{S_0^1(\vec{r}, 0)}{\hbar}\right) + \sqrt{W_2(\vec{r}, 0)} \cos\left(\frac{S_0^2(\vec{r}, 0)}{\hbar}\right)}\right) \quad (32)$$

The amplitude of the combined wave function is the time-evolved density defined in eq. (31), whereas we obtain the phase of the combined wave function:

$$\frac{1}{\hbar}S_0(\vec{R}(t), t) = \frac{1}{\hbar}S_0(\vec{R}(0), 0) + \int_{[P,R]} \vec{P}(t') \cdot \vec{R}(t') - H(\vec{P}(t'), \vec{R}(t')) dt', \quad (33)$$

where the initial momenta are given by

$$\vec{P}(0) = \hbar \vec{\nabla}_{\vec{r}} \text{Im}\left\{\log \psi(\vec{R}(0), t = 0)\right\} = \vec{\nabla}_{\vec{r}} S_0(\vec{R}(0), t = 0). \quad (34)$$

Note that we used here that:

$$\psi(\vec{R}(0), 0) = \sqrt{W(\vec{R}(0), 0)}e^{\frac{i}{\hbar}S_0(\vec{R}(0), 0)} \quad (35)$$

$$\Rightarrow \log \psi = \frac{1}{2} \log W + \frac{i}{\hbar}S_0 + i2\pi k \quad (36)$$

$$\Rightarrow \text{Im}\left\{\log \psi(\vec{R}(0), 0)\right\} = S_0(\vec{R}(0), 0) \quad (37)$$

## Derivation of the method:

First: consider a general Hamilton operator

$$\begin{aligned}\hat{H} &= \frac{1}{2m} \left( \frac{\hbar}{i} \vec{\nabla} - q \vec{A} \right)^2 + \hat{V}(\vec{r}) \\ &= \frac{1}{2m} \sum_i \left( \frac{\hbar}{i} \partial_i - q A_i \right) \left( \frac{\hbar}{i} \partial_i - q A_i \right) + \hat{V}(\vec{r}) \\ &= \frac{1}{2m} \sum_i \left( -\frac{\hbar^2}{i^2} \partial_i^2 - q \frac{\hbar}{i} \partial_i (A_i \cdot \cdot) - q \frac{\hbar}{i} A_i \partial_i + q^2 A_i^2 \right) + \hat{V}(\vec{r}) \\ &= \frac{1}{2m} \left( -\hbar^2 \Delta + q^2 A^2 - q \frac{\hbar}{i} A_i \partial_i - q \frac{\hbar}{i} \partial_i (A_i \cdot \cdot) \right) + \hat{V}(\vec{r})\end{aligned}$$

Now consider:

$$\begin{aligned}\hat{H} e^{\frac{i}{\hbar} S} &= V(\vec{r}) e^{\frac{i}{\hbar} S} + \frac{1}{2m} \left( q^2 A^2 e^{i/\hbar S} - q \frac{\hbar}{i} A_i \left( e^{i/\hbar S} \partial_i + \frac{i}{\hbar} e^{i/\hbar S} \partial_i S \right) \right. \\ &\quad \left. - q \frac{\hbar}{i} \left( e^{i/\hbar S} \partial_i A_i + A_i \frac{i}{\hbar} e^{i/\hbar S} \partial_i S + A_i e^{i/\hbar S} \partial_i \right) \right. \\ &\quad \left. + \left( (\partial_i S)^2 + \frac{\hbar}{i} \partial_i^2 S \right) e^{i/\hbar S} \right)\end{aligned}$$

So

$$\begin{aligned}e^{-\frac{i}{\hbar} S} \hat{H} e^{\frac{i}{\hbar} S} &= \hat{V}(\vec{r}) + \frac{1}{2m} \left( q^2 A^2 - q \frac{\hbar}{i} \frac{i}{\hbar} A_i \partial_i S - q \frac{\hbar}{i} \partial_i A_i - q \frac{\hbar}{i} \frac{i}{\hbar} A_i \partial_i S \right. \\ &\quad \left. + (\partial_i S)^2 + \frac{\hbar}{i} \partial_i^2 S \right) \\ &= V(\vec{r}) + \frac{1}{2m} \left( \underline{q^2 A^2} - \underline{2q A_i \partial_i S} - \underline{q \frac{\hbar}{i} \partial_i A_i} + \underline{(\partial_i S)^2} + \underline{\frac{\hbar}{i} \partial_i^2 S} \right) \\ &= V(\vec{r}) + \frac{1}{2m} \left( \underline{(\partial_i S - q A_i)^2} + \underline{\frac{\hbar}{i} (\partial_i^2 S - q \partial_i A_i)} \right) \\ &= V(\vec{r}) + \frac{1}{2m} \left( (\vec{\nabla}_r S - q \vec{A})^2 + \frac{\hbar}{i} (\vec{\nabla}_r^2 S - q \vec{\nabla}_r \cdot \vec{A}) \right)\end{aligned}$$

Insert this into the Schrödinger equation:

$$\begin{aligned}(i\hbar \partial_t - \hat{H}) \psi &= 0 & \text{Ansatz } \psi &= e^{i/\hbar S} \\ (i\hbar \partial_t - \hat{H}) e^{i/\hbar S} & & \text{multiply from left with } -e^{-i/\hbar S}\end{aligned}$$

$$\boxed{\partial_t S + V(\vec{r}) + \frac{1}{2m} \left( (\vec{\nabla}_r S - q \vec{A})^2 + \frac{\hbar}{i} (\vec{\nabla}_r^2 S - q \vec{\nabla}_r \cdot \vec{A}) \right) = 0} *$$

“The general equation of motion”

Taylor expansion in  $\hbar$ :

$$\text{Ansatz: } S(\vec{r}, t) = \sum_{n=0}^{\infty} \left(\frac{\hbar}{i}\right)^n S_n(\vec{r}, t)$$

goal is to find e.o.m. for  $S_n$ :

• equation for  $S_0$ : set  $\hbar \rightarrow 0$ :

$$\partial_t S_0 + V(\vec{r}) + \frac{1}{2m} (\vec{\nabla}_r S_0 - q \vec{A})^2$$

From now on:  $q = 0$

$$\partial_t S_0 + V(\vec{r}) + \frac{1}{2m} (\vec{\nabla}_r S_0)^2 = 0 \quad \text{with}$$

$$\vec{p} = \vec{\nabla}_r S_0$$

$$\boxed{\partial_t S_0 + H(\vec{p}, \vec{r}) = 0} \quad ①$$

• equation for  $S_1$ :

consider  $\partial_t(\hbar/i) *$  and set  $\hbar \rightarrow 0$ :

$$\cancel{\partial_t \hbar} * : \partial_t S_1 + \frac{1}{2m} \left( \vec{\nabla}_r^2 S_0 + 2\frac{\hbar}{i} \vec{\nabla}_r^2 S_1 + \frac{2\hbar}{i} (\vec{\nabla}_r S_0)^2 + 2(\vec{\nabla}_r S_0)(\vec{\nabla}_r S_1) \right)$$

$$\hbar \rightarrow 0$$

$$\partial_t S_1 + \frac{1}{2m} (\vec{\nabla}_r^2 S_0 + 2(\vec{\nabla}_r S_0)(\vec{\nabla}_r S_1)) = 0$$

$$\partial_t S_1 + \frac{1}{2m} (\vec{\nabla}_r \vec{p} + 2 \vec{p} \vec{\nabla}_r S_1) = 0$$

$$\partial_t S_1 + \frac{\vec{p}}{m} \vec{\nabla}_r S_1 + \frac{1}{2m} \vec{\nabla}_r \vec{p} = 0$$

compare: k.10

$$\boxed{\partial_t S_1 + \frac{\vec{p}}{m} \vec{\nabla}_r S_1 + \frac{1}{2m} \vec{\nabla}_r \vec{p} = 0} \quad ②$$

Let's solve ① and ② with classical trajectories:

Solution for  $S_0$ :

$$\partial_t S_0 + V(\vec{r}) + \frac{1}{2m} (\vec{\nabla}_r S_0)^2 = 0 \quad \text{cannot be solved easily}$$

Consider:

$$\begin{aligned}\frac{d}{dt} S_0(\vec{R}(t), t) &= \gamma_t S_0(\vec{R}(t), t) + \frac{\partial S_0}{\partial \vec{R}} \cdot \dot{\vec{R}} \\ &= \underbrace{\gamma_t S_0(\vec{R}(t), t)}_{-H(\vec{P}, \vec{R})} + \nabla_r S_0(\vec{R}(t), t) \cdot \dot{\vec{R}(t)}\end{aligned}$$

$$\frac{d}{dt} S_0 = \nabla_r S_0 \cdot \dot{\vec{R}} - H(\vec{v}_{S_0}, \vec{R})$$

$$\Rightarrow S_0(\vec{R}(t), t) = \int dt' (\vec{p} \cdot \dot{\vec{p}} - H(\vec{p}, \vec{R})) + S_0(\vec{R}(0), 0)$$

cannot evaluate this integral if  $\vec{p}$  is not known beforehand:

Find:  $\vec{p} = \nabla_r S_0$ ;

$$\vec{p} = \nabla_r S_0(\vec{R}(t), t) = \sum_i \hat{e}_i \gamma_i; S_0(\vec{R}(t), t) = \sum_{ij} \hat{e}_i \gamma_j \underbrace{S_0 \gamma_{ij}}_{\delta_{ij}} = \sum_i \hat{e}_i \gamma_i S_0$$

$$\frac{d\vec{p}}{dt} = \frac{d}{dt} \left( \sum_i \hat{e}_i \gamma_i S_0 \right) = \sum_i \hat{e}_i \left( \gamma_t \gamma_i S_0 + \sum_j \dot{\vec{R}}_j \gamma_j \gamma_i S_0 \right)$$

$$= \sum_i \hat{e}_i \left( \gamma_i \underbrace{\gamma_t S_0}_{-H} + \sum_j \dot{\vec{R}}_j \gamma_j \gamma_i S_0 \right)$$

$$= \sum_{ij} \hat{e}_i \left( -\gamma_j H \underbrace{\gamma_i \gamma_j}_{\delta_{ij}} - \gamma_{pj} H \underbrace{\gamma_i \gamma_j}_{\delta_{ij}} + \dot{\vec{R}}_j \gamma_j \gamma_i S_0 \right)$$

$$= \sum_i -\hat{e}_i \gamma_i H + \sum_{ij} \hat{e}_i \left( -\frac{\partial H}{\partial p_j} + \dot{\vec{R}}_j \right) \gamma_i \gamma_j S_0$$

$$= -\vec{\nabla}_r H + \underbrace{(\dot{\vec{R}} - \vec{\nabla}_p H) \vec{\nabla}_r \otimes \vec{\nabla}_r S_0}$$

choose path s.t. this term is 0, otherwise cannot compute.

$$\vec{\nabla}_r \otimes \vec{\nabla}_r = \begin{pmatrix} \gamma_x (\gamma_x + \gamma_y + \gamma_z) \\ \gamma_x (\gamma_x + \gamma_y + \gamma_z) \\ \gamma_z (\gamma_x + \gamma_y + \gamma_z) \end{pmatrix}$$

Trajectory e.o.m.:

$$\begin{aligned}\dot{\vec{R}} &= \vec{\nabla}_p H(\vec{p}, \vec{R}, t) \\ \dot{\vec{p}} &= -\nabla_r H(\vec{p}, \vec{R}, t)\end{aligned}$$

Solution for  $S_1$ : (based on particle conservation law)

Let  $w(\vec{r}, t)$  be particle density distribution in space. The density moves with a velocity field

$$\vec{v}(\vec{r}, t) = \vec{\nabla}_p H(\vec{p}, \vec{r}, t) |_{\vec{p} = \vec{\nabla}_r S_0}$$

The continuity equation yields:

$$\begin{aligned}\gamma_t \int_S d^3 r w(\vec{r}, t) + \oint_S dA \vec{v}(\vec{r}, t) w(\vec{r}, t) &= 0 \\ \hookrightarrow \gamma_t w(\vec{r}, t) + \vec{\nabla} \cdot (\vec{v}(\vec{r}, t) w(\vec{r}, t)) &= 0\end{aligned}$$

$$\gamma_w(\vec{r}, t) + \vec{\nabla} \cdot \vec{w} + w \vec{\omega} \cdot \vec{v} = 0$$

$$\frac{d}{dt} (w(\vec{R}(t), t)) + w(\vec{R}(t), t) \vec{\nabla} \cdot \vec{v} = 0$$

$$\Leftrightarrow \frac{1}{w(\vec{R}, t)} \frac{d}{dt} (w(\vec{R}(t), t)) = - \vec{\nabla} \cdot \vec{v}$$

$$\frac{1}{dt} \ln w(\vec{R}(t), t) = - \vec{\nabla} \cdot \vec{v} (\vec{R}(t), t) = - \vec{\nabla}_r \cdot \vec{R} = - \vec{\nabla}_r \cdot \vec{\sigma}_p H(\vec{p}, \vec{R}, t)$$

$\underbrace{\vec{R}}_{\vec{v}_p H(\vec{p}, \vec{R}, t)}$

This is the exact equation for  $S_1$ ; reminder:

$$\partial_t S_1 + \frac{\vec{p}}{m} \vec{\nabla}_r S_1 + \frac{1}{2m} \vec{\nabla}_r \cdot \vec{p} = 0$$

$$\Leftrightarrow \gamma_w S_1 + (\vec{\sigma}_p H(\vec{p}, \vec{R}, t)) (\vec{\nabla}_r S_1) + \frac{1}{2} \vec{\nabla}_r \vec{\sigma}_p H(\vec{p}, \vec{R}) = 0$$

$$\Leftrightarrow \gamma_w S_1 = - (\vec{\sigma}_p H(\vec{p}, \vec{R}, t)) (\vec{\nabla}_r S_1) - \frac{1}{2} \vec{\nabla}_r \vec{\sigma}_p H(\vec{p}, \vec{R})$$

Now consider:  $\frac{d}{dt} S_1(\vec{R}(t), t) = \gamma_w S_1(\vec{R}(t), t) + \sum_i \gamma_i S_1(\vec{R}(t), t) \underbrace{\dot{R}_i}_{\vec{\nabla}_p H(\vec{p}, \vec{R}, t)}$

$$= \gamma_w S_1(\vec{R}(t), t) + \vec{\nabla}_r S_1(\vec{R}(t), t) \vec{\sigma}_p H(\vec{p}, \vec{R}, t)$$

$$= - (\vec{\sigma}_p H(\vec{p}, \vec{R}, t)) (\vec{\nabla}_r S_1) - \frac{1}{2} \vec{\nabla}_r \vec{\sigma}_p H(\vec{p}, \vec{R}) + \vec{\nabla}_r S_1(\vec{R}(t), t) \vec{\nabla}_p H(\vec{p}, \vec{R}, t)$$

$$= - \frac{1}{2} \vec{\nabla}_r \vec{\sigma}_p H(\vec{p}, \vec{R}, t)$$

$$\frac{d}{dt} S_1(\vec{R}(t), t) = \frac{1}{2} \frac{d}{dt} \ln (w(\vec{R}, t))$$

$$\hookrightarrow S_1(\vec{R}(t), t) = S_1(\vec{R}(0), 0) + \frac{1}{2} \ln \left( \frac{w(\vec{R}(t), t)}{w(\vec{R}(0), 0)} \right)$$

Initial conditions:

$$\text{Reminder: } \Psi(\vec{r}, t) = \exp \left( \frac{i}{\hbar} (S_0(\vec{r}, t) + \frac{1}{2} S_1(\vec{r}, t)) \right)$$

$$\text{so } \Psi(\vec{r}, t=0) = \exp \left( \frac{i}{\hbar} S_0(\vec{r}, 0) \right) \exp \left( S_1(\vec{r}, 0) \right)$$

Note that  $S_0$  and  $S_1$  are both real:

$$\Rightarrow \ln \Psi(\vec{r}, 0) = \frac{i}{\hbar} S_0(\vec{r}, 0) + S_1(\vec{r}, 0)$$

$$\text{Im} \ln \Psi(\vec{r}, 0) = \frac{1}{\hbar} S_0(\vec{r}, 0)$$

$$\text{Re} \ln \Psi(\vec{r}, 0) = S_1(\vec{r}, 0)$$

$$S_0(\vec{r}, 0) = \text{tr} \ln \ln \Psi(\vec{r}, 0)$$

$$S_1(\vec{r}, 0) = \text{Re} \ln \Psi(\vec{r}, 0)$$

Finally we need initial momentum for a trajectory  $\vec{P}(0)$ :

remember:  $\vec{p} = \vec{\nabla}_r S_0$

$$\text{so } \vec{p}(\vec{r}, t=0) = \text{tr} \vec{\nabla}_r \ln \ln \Psi(\vec{r}, 0)$$

Summary:

$$\Psi(\vec{r}, t) = \exp\left(\frac{i}{\hbar}\left(S_0(\vec{r}, 0) + \int_{[\vec{R}, \vec{p}]} dt (\vec{p} \cdot \dot{\vec{R}} - H(\vec{P}, \vec{R}, t))\right)\right) \exp\left(S_1(\vec{r}, 0) + \frac{1}{2} \ln\left(\frac{w(\vec{R}(t), t)}{w(\vec{R}(0), 0)}\right)\right)$$

$$= \exp\left(\frac{i}{\hbar} \text{tr} \ln \ln \Psi(\vec{r}, 0)\right) \exp\left(\frac{i}{\hbar} \int_{[\vec{P}, \vec{R}]} dt L(P, R)\right) \exp(\text{Re} \ln \Psi(\vec{r}, 0)) \\ \cdot \sqrt{\frac{w(\vec{R}(t), t)}{w(\vec{R}(0), 0)}}.$$

$$\Psi(\vec{r}, t) = \sqrt{\frac{w(\vec{R}(t), t)}{w(\vec{R}(0), 0)}} \underbrace{\exp(\text{Re} \ln \Psi(\vec{r}, 0) + i \ln \ln \Psi(\vec{r}, 0))}_{\Psi(\vec{r}, t=0)} \\ \cdot \exp\left(\frac{i}{\hbar} \int_{[\vec{R}, \vec{p}]} dt L(\vec{P}, \vec{R})\right)$$

$$\text{Set } w(\vec{R}(0), t=0) = |\Psi(\vec{R}(0), t=0)|^2 \quad , \quad \frac{\Psi}{|\Psi|} = \frac{|\Psi|}{|\Psi|} e^{i \arg \Psi}$$

$$\Psi(\vec{r}, t) = \frac{\Psi(\vec{r}, t=0)}{|\Psi(\vec{r}, t=0)|} \cdot \sqrt{w(\vec{r}, t)} \cdot \exp\left(\frac{i}{\hbar} \int_{[\vec{R}, \vec{p}]} dt [\vec{P} \cdot \dot{\vec{R}} - H(\vec{P}, \vec{R}, t)]\right)$$

The semi-classical approximation

$$\Psi(\vec{r}, t) = \sqrt{w(\vec{r}, t)} \cdot \exp\left(\frac{i}{\hbar} \int_{[\vec{R}, \vec{p}]} dt [\vec{P} \cdot \dot{\vec{R}} - H(\vec{P}, \vec{R}, t)] + i \arg \{\Psi(\vec{R}(0), 0)\}\right)$$

where  $[\vec{R}, \vec{p}]$  is the classical trajectory that starts at  $\vec{R}(0), \vec{p}(0) = \vec{\nabla}_r \ln \ln \Psi(\vec{R}(0), t=0)$

and ends at the point  $\vec{r}$  at time  $t$ .

$$\text{And } w(\vec{r}, t=0) = |\Psi(\vec{r}, t=0)|^2$$

## Example: Simple harmonic oscillator

### 3D-Harmonic oscillator:

$$L = \frac{m}{2} (\dot{x}^2 + \dot{y}^2 + \dot{z}^2) - \frac{k}{2} (x^2 + y^2 + z^2)$$

$$P_x = \frac{\partial L}{\partial \dot{x}} = m \dot{x}, P_y = m \dot{y}, P_z = m \dot{z} \Rightarrow \dot{x}_i = \frac{P_i}{m}$$

$$H(P, q) = \sum_i P_i \dot{q}_i - L = \sum_i m \dot{x}_i^2 - \frac{m}{2} \sum_i \dot{x}_i^2 + \frac{k}{2} \sum_i x_i^2$$

$$H(P, q) = \frac{m}{2} \sum_i \dot{x}_i^2 + \frac{k}{2} \sum_i x_i^2$$

$$H(P, q) = \frac{1}{2m} \sum_i P_i^2 + \frac{k}{2} \sum_i x_i^2, \text{ Let } k = m\omega^2$$

$$H(P, q) = \frac{1}{2m} \sum_i P_i^2 + \frac{1}{2} m \sum_i \omega_i^2 q_i^2$$

### E.O.N.:

$$\begin{aligned} \dot{P}_i &= \frac{\partial H}{\partial q_i} = -m\omega_i^2 q_i \\ \ddot{q}_i &= \frac{\partial H}{\partial P_i} = \frac{P_i}{m} \end{aligned} \quad \left. \begin{array}{l} \\ \end{array} \right\} \ddot{q}_i = -\omega_i^2 q_i$$

known solution

$$\left. \begin{array}{l} x_i(t) = x_{i0} \cos(\omega_i t) + \frac{P_{i0}}{m\omega_i} \sin(\omega_i t) \\ P_i(t) = P_{i0} \cos(\omega_i t) - m\omega_i x_{i0} \sin(\omega_i t) \end{array} \right\} \Rightarrow x_{i0} = \frac{x_i}{\cos(\omega_i t)} - \frac{P_{i0}}{m\omega_i} \tan(\omega_i t)$$

### Action:

$$\begin{aligned} S_0 &= \int L dt = \int_0^t dt \left[ \frac{m}{2} (\dot{x}_i^2 + \dot{y}_i^2 + \dot{z}_i^2) - \frac{1}{2} m \omega_i^2 (x_i^2 + y_i^2 + z_i^2) \right] \\ &= \int_0^t \frac{m}{2} \sum_i \left( \frac{P_{i0}}{m} \cos(\omega_i t) - \omega_i x_{i0} \sin(\omega_i t) \right)^2 - \frac{1}{2} m \omega_i^2 \sum_i \left( x_{i0} \cos(\omega_i t) + \frac{P_{i0}}{m\omega_i} \sin(\omega_i t) \right)^2 \\ &= \int_0^t dt \sum_i \frac{m}{2} \left( \frac{P_{i0}^2}{m^2} \cos^2(\omega_i t) + \omega_i^2 x_{i0}^2 \sin^2(\omega_i t) - \omega_i \frac{P_{i0} x_{i0}}{m} \sin(2\omega_i t) \right) \\ &\quad - \frac{1}{2} m \omega_i^2 \left( x_{i0}^2 \cos^2(\omega_i t) + \frac{P_{i0}^2}{m^2 \omega_i^2} \sin^2(\omega_i t) + x_{i0} P_{i0} \frac{\sin(2\omega_i t)}{m\omega_i} \right) \\ &= \int_0^t dt \sum_i \left( \frac{P_{i0}^2}{2m} \cos^2(\omega_i t) + \frac{m}{2} \omega_i^2 x_{i0}^2 \sin^2(\omega_i t) - \omega_i \frac{P_{i0} x_{i0}}{2} \sin(2\omega_i t) \right) \\ &\quad + \left( -\frac{1}{2} m \omega_i^2 x_{i0}^2 \cos^2(\omega_i t) - \frac{P_{i0}^2}{2m} \sin^2(\omega_i t) - \frac{\omega_i}{2} x_{i0} P_{i0} \sin(2\omega_i t) \right) \\ &= \int_0^t dt \sum_i \frac{P_{i0}^2}{2m} \cos(2\omega_i t) - \frac{1}{2} m \omega_i^2 x_{i0}^2 \cos(2\omega_i t) - \omega_i P_{i0} x_{i0} \sin(2\omega_i t) \\ &= \sum_i \frac{P_{i0}^2}{2m} \frac{\sin(2\omega_i t)}{2\omega_i} - \frac{1}{2} m \omega_i^2 x_{i0}^2 \frac{\sin(2\omega_i t)}{2\omega_i} + \frac{P_{i0} x_{i0}}{2} \left[ \cos(2\omega_i t) - 1 \right] \end{aligned}$$

$$= \sum_i \left[ \frac{p_{io}^2}{2m} - \frac{1}{2} m \omega_i^2 x_{io}^2 \right] \frac{\sin(2\omega_i t)}{2\omega} + \frac{p_{io} x_{io}}{2} \left[ \cos(2\omega_i t) - 1 \right]$$

Insert initial condition  $x_{i0}$ :

$$x_{i0} = \frac{x_i}{\cos(\omega_i t)} - \frac{p_{io}}{m\omega_i} \tan(\omega_i t)$$

$$\begin{aligned} x_{i0}^2 &= \left( \frac{x_i}{\cos(\omega_i t)} - \frac{p_{io}}{m\omega_i} \tan(\omega_i t) \right)^2 = \frac{x_i^2}{\cos^2(\omega_i t)} + \frac{p_{io}^2}{m^2\omega_i^2} \tan^2(\omega_i t) - 2 x_i \frac{p_{io}}{m\omega_i} \frac{\tan(\omega_i t)}{\cos(\omega_i t)} \\ &= \frac{1}{\cos^2(\omega_i t)} \left( x_i^2 + \frac{p_{io}^2}{m^2\omega_i^2} \sin^2(\omega_i t) - 2 x_i \frac{p_{io}}{m\omega_i} \sin(\omega_i t) \right) \end{aligned}$$

$$\Rightarrow S_0(\vec{r}, t) = \sum_i \left[ \frac{p_{io}^2}{2m} - \frac{1}{2} m \omega_i^2 x_{i0}^2 \right] \frac{\sin(\omega_i t) \cos(\omega_i t)}{\omega_i} + \frac{p_{io} x_{i0}}{2} \left[ \cos(2\omega_i t) - 1 \right]$$

$$\begin{aligned} &= \sum_i \frac{p_{io}^2}{2m} \frac{\sin(2\omega_i t)}{2\omega_i} - \frac{1}{2} m \omega_i \tan(\omega_i t) x_i^2 - \frac{p_{io}^2}{2m\omega_i} \frac{\sin^3(\omega_i t)}{\cos(\omega_i t)} + x_i p_{io} \frac{\sin^2(\omega_i t)}{\cos(\omega_i t)} \\ &\quad + \frac{p_{io} x_i}{2 \cos(\omega_i t)} - \frac{p_{io}^2}{2m\omega_i} \tan(\omega_i t) \left[ \cos(2\omega_i t) - 1 \right] \end{aligned}$$

$$\begin{aligned} &= \sum_i \frac{p_{io}^2}{2m} \frac{\sin(2\omega_i t)}{2\omega_i} - \frac{1}{2} m \omega_i \tan(\omega_i t) x_i^2 - \frac{p_{io}^2}{2m\omega_i} \frac{\sin^3(\omega_i t)}{\cos(\omega_i t)} + x_i p_{io} \frac{\sin^2(\omega_i t)}{\cos(\omega_i t)} \\ &\quad - p_{io} x_i \frac{\sin^2(\omega_i t)}{\cos(\omega_i t)} + \frac{p_{io}^2}{m\omega_i} \frac{\sin^3(\omega_i t)}{\cos(\omega_i t)} \end{aligned}$$

$$= \sum_i \frac{p_{io}^2}{2m} \frac{\sin(2\omega_i t)}{2\omega_i} - \frac{1}{2} m \omega_i \tan(\omega_i t) x_i^2 + \frac{p_{io}^2}{2m\omega_i} \frac{\sin^3(\omega_i t)}{\cos(\omega_i t)}$$

$$= \sum_i \frac{p_{io}^2}{2m\omega_i} \left( \sin(\omega_i t) \cos(\omega_i t) + \frac{\sin^3(\omega_i t)}{\cos(\omega_i t)} \right) - \frac{1}{2} m \omega_i \tan(\omega_i t) x_i^2$$

$$= \sum_i \frac{p_{io}^2}{2m\omega_i} \left( \frac{\sin(\omega_i t) \cos^2(\omega_i t) + \sin^3(\omega_i t)}{\cos(\omega_i t)} \right) - \frac{1}{2} m \omega_i \tan(\omega_i t) x_i^2$$

$$= \sum_i \left[ \frac{p_{io}^2}{2m\omega_i} - \frac{1}{2} m \omega_i x_i^2 \right] \tan(\omega_i t)$$

$$\boxed{\int dt \left[ \vec{p} \cdot \dot{\vec{R}} - H(\vec{p}, \vec{R}, t) \right] = \sum_i \left[ \frac{p_{io}^2}{2m\omega_i} - \frac{1}{2} m \omega_i x_i^2 \right] \tan(\omega_i t)}$$

The next section concerns the 1d case:  $H(p, x) = \frac{p^2}{2m} + \frac{1}{2} m \omega^2 x$

Let

$$\varphi(x, t=0) = \sqrt{\frac{|\lambda|}{\sqrt{\pi/2}}} e^{-\lambda^2 (x - \bar{x})^2} e^{\frac{i}{\hbar} p_0 x} \Big|_{p(0) = \hbar \partial_x \ln \ln \varphi(x, 0) = p_0, \arg \varphi(x, t=0) = p_0 x / \hbar}$$

Find  $w(x, t)$ :

Analytical method:

$$w(x, t) = \int dp \, p(x, p, t)$$

$$\text{with } p(x, p, t=0) = w(x) \delta(p - p_0), \quad w(x) = \frac{e^{-2\lambda^2(x - \bar{x})^2}}{\sqrt{\pi/2}} \frac{|\lambda|}{|\lambda|}$$

$$\text{and } \frac{d}{dt} p(x, p, t) = \{ H, p \}$$

$$\text{i.e. } \frac{d}{dt} p(x, p, t) = \frac{\partial H}{\partial x} \frac{\partial p}{\partial p} - \frac{\partial H}{\partial p} \frac{\partial p}{\partial x} \quad \textcircled{1}$$

We can solve this using the method of characteristics.

In general our PDE is equivalent to

$$\frac{d}{ds} p(x(s), p(s)) = 0 \quad \text{along a curve } (x(s), p(s))$$

$$\frac{d}{ds} p = \frac{\partial p}{\partial x} \frac{\partial x}{\partial s} + \frac{\partial p}{\partial p} \frac{\partial p}{\partial s}$$

If we choose:

$$\textcircled{2} \quad \left\{ \begin{array}{l} \frac{\partial x}{\partial s} = -\frac{\partial H}{\partial p} \\ \frac{\partial p}{\partial s} = \frac{\partial H}{\partial x} \\ \text{, 't = s'} \end{array} \right\} \Rightarrow \frac{d}{ds} p = -\frac{\partial H}{\partial p} \frac{\partial p}{\partial x} + \frac{\partial p}{\partial p} \frac{\partial H}{\partial x} \stackrel{!}{=} 0$$

same equation as \textcircled{1}.

So along curves  $(x(s), p(s))$ , the function  $p$  is constant.

$\Rightarrow$  Given a point  $(x, p, t)$  we need to find the initial conditions  $(x_0, p_0, 0)$

that evolve to  $(x, p, t)$  according to \textcircled{2}

$$\Leftrightarrow p(x, p, t) = p(x_0, p_0, 0)$$

\textcircled{2} are just the classical Hamilton equations that have the solution

$$\left\{ \begin{array}{l} x(t) = x_0 \cos(\omega t) + \frac{p_0}{m\omega} \sin(\omega t) \\ p(t) = p_0 \cos(\omega t) - m\omega x_0 \sin(\omega t) \end{array} \right\} \quad \text{We solve these for } x_0(x, p), p_0(x, p)$$

$$\Rightarrow \begin{cases} x_0 = \frac{x(t)}{\cos(\omega t)} - \frac{p_0}{m\omega} \frac{\sin(\omega t)}{\cos(\omega t)} \\ p_0 = \frac{p(t)}{\cos(\omega t)} + m\omega x_0 - \frac{\sin(\omega t)}{\cos(\omega t)} \end{cases}$$

$$\begin{aligned} &\Rightarrow x_0 = \frac{x(t)}{\cos(\omega t)} - \frac{1}{m\omega} \frac{\sin(\omega t)}{\cos(\omega t)} \left( \frac{p(t)}{\cos(\omega t)} + m\omega x_0 - \frac{\sin(\omega t)}{\cos(\omega t)} \right) \\ &\text{substitute } p_0 \text{ in } x_0 \\ &\quad \underbrace{(1 + \tan^2(\omega t))}_{1/\cos^2(\omega t)} x_0 = \frac{x(t)}{\cos(\omega t)} - \frac{1}{m\omega} \frac{\sin(\omega t)}{\cos^2(\omega t)} p(t) \end{aligned}$$

$$\Leftrightarrow x_0 = x(t) \cos(\omega t) - \frac{1}{m\omega} \sin(\omega t) p(t)$$

$$\Rightarrow p_0 = \frac{p}{\cos(\omega t)} + m\omega \tan(\omega t) \left( \frac{x}{\cos(\omega t)} - \frac{p_0}{m\omega} \frac{\sin(\omega t)}{\cos(\omega t)} \right)$$

$$\text{substitute } x_0 \text{ in } p_0 \\ (1 + \tan^2(\omega t)) p_0 = \frac{p}{\cos(\omega t)} + m\omega \tan(\omega t) \frac{x}{\cos(\omega t)}$$

$$\Rightarrow \begin{cases} x_0 = x \cos(\omega t) - \frac{1}{m\omega} \sin(\omega t) p \\ p_0 = p \cos(\omega t) + m\omega \sin(\omega t) x \end{cases}$$

Now we obtain  $f(x, p, t)$ :

$$\begin{aligned} f(x, p, t) &= f(x = x_0, p = p_0, t = 0) \\ &= W(x \cos(\omega t) - \frac{1}{m\omega} \sin(\omega t) p) \delta(p \cos(\omega t) + m\omega \sin(\omega t) x - p_0). \end{aligned}$$

To obtain  $\omega(x, t)$  use  $\omega(x, t) = \int dp f(x, p, t)$  and the properties of  $\delta$ :

$$\delta(f(p)) = \frac{1}{|f'(p)|} \delta(p-h) \text{ where } h \text{ is a zero of } f.$$

$$\begin{aligned} W(x, t) &= \int dp W(x \cos(\omega t) - \frac{1}{m\omega} \sin(\omega t) p) \delta(p \cos(\omega t) + m\omega \sin(\omega t) x - p_0) \\ &= \int dp \frac{1}{|\cos \omega t|} W(x \cos(\omega t) - \frac{1}{m\omega} \sin(\omega t) p) \delta(p - \frac{p_0 - m\omega \sin \omega t x}{\cos \omega t}) \\ &= \frac{1}{|\cos \omega t|} W\left(x \cos(\omega t) - \frac{1}{m\omega} \sin(\omega t) \frac{p_0 - m\omega \sin \omega t x}{\cos \omega t}\right) \\ &= \frac{1}{|\cos \omega t|} W\left(x \cos(\omega t) - \frac{p_0}{m\omega} \tan \omega t + x \frac{\sin^2 \omega t}{\cos \omega t}\right) \\ &= \frac{1}{|\cos \omega t|} W\left(\frac{x}{\cos \omega t} - \frac{p_0}{m\omega} \tan \omega t\right) \end{aligned}$$

Substituting the original form of  $W$ , we obtain:

$$W(x, t) = \frac{1}{\sqrt{\pi/2}} \left| \frac{\lambda}{\cos(\omega t)} \right| \exp \left\{ -2\lambda^2 \left( \frac{x}{\cos \omega t} - \frac{1}{m\omega} \tan \omega t P_0 - \bar{x} \right)^2 \right\}.$$

### Sanity checks :

i) Numerical simulation: initialize lots of walkers with  $x_0 \sim W(x_0)$

and let their trajectories evolve classically. Track their distribution with time and compare with  $W(x, t)$ .

(see Notebook: density.ipynb) results match exactly! ✓

ii)  $W(x, t)$  is normalized  $\forall t$ :

$$\begin{aligned} \int dx W(x, t) &= \frac{1}{\sqrt{\pi/2}} \left| \frac{\lambda}{\cos(\omega t)} \right| \int \exp \left\{ -2\lambda^2 \left( \frac{x}{\cos \omega t} - \frac{1}{m\omega} \tan \omega t P_0 - \bar{x} \right)^2 \right\} dx \\ &= \frac{1}{\sqrt{\pi/2}} \left| \frac{\lambda}{\cos(\omega t)} \right| \int \exp \left\{ -\frac{2\lambda^2}{(\cos \omega t)^2} \left( x - \frac{1}{m\omega} \frac{\tan \omega t}{\cos \omega t} P_0 - \bar{x} \right)^2 \right\} dx \\ &= \frac{1}{\sqrt{\pi/2}} \left| \frac{\lambda}{\cos(\omega t)} \right| \sqrt{\frac{\pi (\cos \omega t)^2}{2\lambda^2}} = 1. \quad \checkmark \end{aligned}$$

iii)  $f(x, p, t)$  solves the Liouville equation:

$$f(x, p, t) = W \left( x \cos(\omega t) - \frac{1}{m\omega} \sin(\omega t) p \right) \delta(p \cos(\omega t) + m\omega \sin(\omega t) x - p_0)$$

$$\begin{aligned} \bullet \frac{1}{\omega} \frac{\partial f}{\partial x} &= -2\lambda^2 \cos(\omega t) \left( x \cos \omega t - \frac{1}{m\omega} \sin \omega t p \right) \delta(p \cos \omega t + m\omega \sin \omega t x - p_0) \\ &\quad + \delta'(p \cos \omega t + m\omega \sin \omega t x - p_0) m\omega \sin \omega t \end{aligned}$$

$$\begin{aligned} \bullet \frac{1}{\omega} \frac{\partial f}{\partial p} &= \frac{2\lambda^2}{m\omega} \sin(\omega t) \left( x \cos \omega t - \frac{1}{m\omega} \sin \omega t p \right) \delta(p \cos \omega t + m\omega \sin \omega t x - p_0) \\ &\quad + \delta'(p \cos \omega t + m\omega \sin \omega t x - p_0) \cdot \cos \omega t \end{aligned}$$

$$\begin{aligned} \bullet \frac{1}{\omega} \frac{\partial f}{\partial t} &= -2\lambda^2 \left( -x\omega \sin(\omega t) - \frac{p}{m} \cos(\omega t) \right) \left( x \cos \omega t - \frac{1}{m\omega} \sin \omega t p \right) \delta(p \cos \omega t + m\omega \sin \omega t x - p_0) \\ &\quad + \delta'(p \cos \omega t + m\omega \sin \omega t x - p_0) (-p\omega \sin \omega t + m\omega^2 \cos \omega t x) \end{aligned}$$

$$\frac{1}{m} \frac{\partial f}{\partial t} = \frac{1}{m} \left( \frac{\partial H}{\partial x} \frac{\partial f}{\partial p} - \frac{\partial H}{\partial p} \frac{\partial f}{\partial x} \right) .$$

With  $H(p, x) = \frac{p^2}{2m} + \frac{1}{2} m \omega^2 x^2$ ,  $\frac{\partial H}{\partial x} = m \omega^2 x$ ;  $\frac{\partial H}{\partial p} = \frac{p}{m}$ .

R.H.S:

$$\begin{aligned} & \frac{2\lambda^2}{m\omega} \sin(\omega t) \left( x \cos(\omega t) - \frac{1}{m\omega} \sin(\omega t) p \right) \delta(p \cos(\omega t) + m\omega \sin(\omega t) x - p_0) m \omega^2 x \\ & + \delta'(p \cos(\omega t) + m\omega \sin(\omega t) x - p_0) \cdot \cos(\omega t) m \omega^2 x \\ & + 2\lambda^2 \cos(\omega t) \left( x \cos(\omega t) - \frac{1}{m\omega} \sin(\omega t) p \right) \delta(p \cos(\omega t) + m\omega \sin(\omega t) x - p_0) \frac{p}{m} \\ & - \delta'(p \cos(\omega t) + m\omega \sin(\omega t) x - p_0) m \omega \sin(\omega t) \frac{p}{m} \\ = & 2\lambda^2 \left( x \cos(\omega t) - \frac{1}{m\omega} \sin(\omega t) p \right) \delta \cdot \left( \sin(\omega t) \omega x + \frac{p}{m} \cos(\omega t) \right) \\ & + \delta' \cdot (m \omega^2 x \cos(\omega t) - \omega \sin(\omega t) p) \\ \stackrel{?}{=} & L.H.S. \quad 2\lambda^2 \left( x \cos(\omega t) - \frac{1}{m\omega} \sin(\omega t) p \right) \delta \cdot \left( x \omega \sin(\omega t) + \frac{p}{m} \cos(\omega t) \right) \\ & + \delta' \cdot (m \omega^2 x \cos(\omega t) - p \omega \sin(\omega t)) \quad \checkmark \end{aligned}$$

IV) This is equivalent to tracing the trajectories: (analytical derivation)

Compare to Ansatz:  $w(x, t) = \frac{1}{N} \sum_j \delta(x - x_j(t))$ , with  $\frac{1}{N} \sum_j \delta(x - x_j(0)) = w(x, 0)$

$$w(x, p, 0) = w(x, 0) \delta(p - p_0) = \frac{1}{N} \sum_j \delta(x - x_j(0)) \cdot \delta(p - p_0)$$

Solution for  $\delta(x, p, t) = \delta(x = x_0, p = p_0, t = 0)$

$$= \frac{1}{N} \sum_j \delta(x \cos(\omega t) - \frac{1}{m\omega} \sin(\omega t) p - x_j(0)) \delta(p \cos(\omega t) + m\omega \sin(\omega t) x - p_0)$$

$$\int dp \Rightarrow w(x, t) = \frac{1}{N} \sum_j \frac{1}{|\cos(\omega t)|} \delta \left( \frac{x}{\cos(\omega t)} - \frac{p_0}{m\omega} \tan(\omega t) - x_j(0) \right)$$

$$= \frac{1}{N} \sum_j \frac{|\cos(\omega t)|}{|\cos(\omega t)|} \delta \left( x - \left( x_j(0) \cos(\omega t) + \frac{p_0}{m\omega} \sin(\omega t) \right) \right)$$

$x_j(t)$

$$= \frac{1}{N} \sum_j \delta(x - x_j(t)) .$$

## Discussion:

- This ansatz requires reverse engineering the trajectory:

input  $x, t \rightarrow$  find  $x_0$  s.t.  $x(t) = x$  and  $x(t=0) = x_0$

- Is this computationally efficient?

- How does integrating over  $p$  work numerically?

↳ solve  $p(t) - p_0 = 0$  for  $p(0)$  and substitute in  $x(t)$ , divide by  $(p'(t))$

- The Ansatz  $w(x,t) = \frac{w(x,0) \cdot v(0)}{v(t)}$  must be wrong. The argument of

$w(x,0)$  cannot include  $x/\cos \omega t$  at all.

- Previous results probably lack large enough number of walkers.

Still unclear.

The final solution of the harmonic oscillator in the semi-classical limit:

$$\psi(x,t) = \sqrt{\frac{1}{\pi(1/2)}} \left| \frac{\lambda}{\cos(\omega t)} \right|^{\frac{1}{2}} \exp \left\{ -\lambda^2 \left( \frac{x}{\cos(\omega t)} - \frac{\tan(\omega t)}{m\omega} p_0 - \bar{x} \right)^2 + i \frac{p_0 x}{\hbar} + \frac{i}{\hbar} \left[ \frac{p_0^2}{2m\omega} - \frac{1}{2} m\omega x^2 \right] \tan(\omega t) \right\}$$

## Quantum harmonic oscillator:

$$\Psi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} \frac{1}{\sqrt{2^n n!}} H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right) e^{-\frac{1}{2} \frac{m\omega}{\hbar} x^2}$$

$$E_n = \hbar\omega(n + \frac{1}{2})$$

Task: find  $\psi(x, t)$  given  $\psi(x, t=0) = e^{-\lambda^2(x-\bar{x})} e^{i\frac{p_0 x}{\hbar}}$

Solution:

$$|\psi(t)\rangle = e^{-\frac{i}{\hbar} \hat{H}t} |\psi(0)\rangle = \sum_{n=0}^{\infty} e^{-\frac{i}{\hbar} \hat{H}t} |n\rangle \langle n| \psi(0)\rangle \\ = \sum_{n=0}^{\infty} e^{-\frac{i}{\hbar} E_n t} \langle n| \psi(0)\rangle |n\rangle .$$

Find:  $\langle n | \psi(0)\rangle = \int dx \left( \left( \frac{m\omega}{\pi\hbar} \right)^{\frac{1}{4}} \frac{1}{\sqrt{2^n n!}} H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right) e^{-\frac{1}{2} \frac{m\omega}{\hbar} x^2} e^{-\lambda^2(x-\bar{x})} e^{i\frac{p_0 x}{\hbar}} \right)$

$$= \int dx \frac{1}{\sqrt{\epsilon}} H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right) e^{-\frac{1}{2} \frac{m\omega}{\hbar} x^2} e^{-\lambda^2(x-\bar{x})} e^{i\frac{p_0 x}{\hbar}}$$

$$= \int dx \frac{1}{\sqrt{\epsilon}} H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right) \exp \left\{ - \left( \lambda^2 x^2 - 2\lambda^2 x \bar{x} + \lambda^2 \bar{x}^2 + \frac{1}{2} \frac{m\omega}{\hbar} x^2 - i \frac{p_0 x}{\hbar} \right) \right\}$$

$$= \int dx \frac{1}{\sqrt{\epsilon}} H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right) \exp \left\{ - \left( \underbrace{x^2 (\lambda^2 + \frac{1}{2} \frac{m\omega}{\hbar})}_{\alpha} - x \underbrace{(2\lambda \bar{x} + i \frac{p_0}{\hbar})}_{\beta} + \underbrace{\lambda^2 \bar{x}^2}_{\gamma} \right) \right\}$$

$$= \int dx \frac{1}{\sqrt{\epsilon}} H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right) \exp \left\{ - \left( \alpha x^2 - \beta x + \gamma \right) \right\}$$

$$= \int dx \frac{1}{\sqrt{\epsilon}} H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right) \exp \left\{ - \alpha \left( x^2 - \frac{b}{a} x + \left(\frac{b}{2a}\right)^2 + \frac{c}{a} - \left(\frac{b}{2a}\right)^2 \right) \right\}$$

$$= \int dx \frac{1}{\sqrt{\epsilon}} H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right) \exp \left\{ - \alpha \left( x - \frac{b}{2a} \right)^2 - c + \frac{b^2}{4a} \right\}$$

$$= \frac{1}{\sqrt{\epsilon}} e^{-c + \frac{b^2}{4a}} \int dx H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right) \exp \left\{ - \alpha \left( x - \frac{b}{2a} \right)^2 \right\} \circ$$

How to solve  $\int H_n(\alpha x) e^{-\alpha(x - \frac{b}{2a})^2} dx$

Use generating function:  $F(x, t) = e^{2\alpha xt - t^2} = \sum_{n=0}^{\infty} \frac{t^n}{n!} H_n(\alpha x)$

Consider:  $\int F(x, t) e^{-\alpha(x - \frac{b}{2a})^2} dx = \int dx e^{2\alpha xt - t^2} e^{-\alpha(x - \frac{b}{2a})^2}$

$$= \int dx \exp \left\{ -\alpha \left[ x^2 - \underbrace{\frac{b+2\alpha t}{\alpha} x + \left(\frac{b+2\alpha t}{2a}\right)^2}_{\beta} + \frac{t^2}{\alpha} + \frac{b^2}{4a^2} - \left(\frac{b+2\alpha t}{2a}\right)^2 \right] \right\}$$

$$= \int dx \exp \left\{ -\alpha (x - \beta/2)^2 \right\} \exp \left\{ -\alpha \left( \frac{t^2}{\alpha} + \frac{b^2}{4a^2} - \frac{(b+2\alpha t)^2}{(2a)^2} \right) \right\}$$

$$= \int dx \exp \left\{ -\alpha (x - \beta/2)^2 \right\} \exp \left( -t^2 - \frac{b^2}{4a} + \frac{b^2 + 4\alpha b t + 4\alpha^2 t^2}{4a} \right)$$

$$= \int dx \exp \left\{ -\alpha (x - \beta/\omega)^2 \right\} \exp \left( \frac{-\alpha t^2 \omega b t + \alpha^2 t^2}{\alpha} \right)$$

$$= \sqrt{\frac{\pi}{\alpha}} \exp \left\{ \underbrace{\left( \frac{\alpha^2 - \alpha}{\alpha} \right) t^2}_{S} + \underbrace{\frac{\alpha b}{\alpha} t}_{k} \right\} := G(t)$$

On the other hand:

$$\int F(x,t) e^{-\alpha(x-\frac{b}{2\omega})^2} dx = \sum_{n=0}^{\infty} \frac{t^n}{n!} \int dx H_n(\alpha x) e^{-\alpha(x-\frac{b}{2\omega})^2}$$

$$so \quad \frac{d^k}{dt^k} G(t) = \sum_{n=0}^{\infty} t^{n-k} \binom{n}{k} \frac{k!}{n!} \int dx H_n(\alpha x) e^{-\alpha(x-\frac{b}{2\omega})^2} \quad \text{Note } \frac{\prod_{i=0}^k (n-i)}{n!} = \binom{n}{k} \frac{k!}{n!}$$

And

$$\frac{d^n}{dt^n} G(t=0) = \int dx H_n(\alpha x) e^{-\alpha(x-\frac{b}{2\omega})^2}.$$

How to evaluate that?

$$\frac{d}{dt} G(t) = G(t) \cdot (2st + k), \quad \frac{d^2}{dt^2} G(t) = G'(t) (2st + k) + G(t) \cdot (2s),$$

$$\frac{d^3}{dt^3} G(t) = (2s) G'(t) + G''(t) (2st + k) + G'(t) \cdot (2s) = (2) \cdot (2s) G'(t) + (2st + k) G''(t)$$

$$\text{General formula: } G^{(n)}(t) = (n-1)(2s) G^{(n-2)}(t) + (2st + k) G^{(n-1)}(t)$$

$$\begin{aligned} \text{Proof per induction } \frac{d}{dt} G^{(n)}(t) &= (n-1) \cdot 2s G^{(n-1)}(t) + (2st + k) G^n(t) + 2s G^{(n-1)} \\ &= n \cdot 2s G^{(n-1)}(t) + (2st + k) G^n(t) = G^{(n+1)}(t) \end{aligned}$$

Find time evolution numerically:

We cannot evaluate infinite sum, so do it up to  $n$ -cutoff, determined when including extra terms, doesn't affect result much.

In total we have:

$$\psi(x,t) = \sum_{n=0}^{\infty} e^{-i \frac{E_n t}{\hbar}} \langle n | \psi(0) \rangle \langle x | n \rangle$$

$$\psi_n(x) = \left( \frac{m\omega}{\pi\hbar} \right)^{\frac{1}{4}} \frac{1}{\sqrt{2^n n!}} H_n \left( \sqrt{\frac{m\omega}{\hbar}} x \right) e^{-\frac{1}{2} \frac{m\omega}{\hbar} x^2}$$

$$E_n = \hbar\omega(n + \frac{1}{2})$$

$$\langle n | \psi(0) \rangle = \left( \frac{m\omega}{\pi\hbar} \right)^{\frac{1}{4}} \frac{1}{\sqrt{2^n n!}} e^{(-c + \frac{b^2}{4\alpha})} \frac{d^n}{dt^n} G(t=0)$$

$$\text{with } G(t) = \sqrt{\frac{\pi}{\alpha}} e^{st^2 + kt}, \quad G^n(t) = 2s(n-1) G^{(n-2)}(t) + kst + k G^{(n-1)}(t)$$

$$s = \frac{\alpha^2 - \alpha}{\alpha}, \quad k = \frac{\alpha b}{\alpha}, \quad \alpha = \sqrt{\frac{m\omega}{\hbar}}$$

$$a = (\lambda^2 + \frac{1}{2} \frac{m\omega}{\hbar}), \quad b = (2\lambda\bar{x} + \frac{iP_0}{\hbar}), \quad c = \lambda^2 \bar{x}^2$$

Quantum harmonic oscillator in 3D:

$$\Psi(\vec{x}, t=0) = e^{i \frac{\vec{p}^T \vec{x}}{\hbar}} e^{-\frac{1}{2} (\vec{x} - \vec{\theta})^T \Sigma^{-1} (\vec{x} - \vec{\theta})}, \quad \omega_i = \sqrt{\frac{m\omega_i}{\hbar}} \quad \underline{\omega} = \begin{pmatrix} \omega_1 & \omega_2 & \omega_3 \end{pmatrix}$$

$$\Psi_{n_1 n_2 n_3}(x, y, z) = \frac{1}{z} e^{-\frac{1}{2} \vec{x}^T \underline{\omega} \vec{x}} H_{n_1}(\alpha_1 x_1) H_{n_2}(\alpha_2 x_2) H_{n_3}(\alpha_3 x_3)$$

Find  $\langle n_1 n_2 n_3 | \Psi(0) \rangle$ :

$$\text{Consider: } F(x_i, t_i) = \sum_{n=0}^{\infty} \frac{t_i^n}{n!} H_n(\alpha_i x_i),$$

$$\text{and } \prod_{i=1}^3 F(x_i, t_i) = \sum_{n_1, n_2, n_3=0}^{\infty} \frac{t_1^{n_1}}{n_1!} \frac{t_2^{n_2}}{n_2!} \frac{t_3^{n_3}}{n_3!} H_{n_1}(\alpha_1 x_1) H_{n_2}(\alpha_2 x_2) H_{n_3}(\alpha_3 x_3)$$

$$= \exp\left(\sum_{i=1}^3 2\alpha_i x_i t_i - t_i^2\right) = e^{-3t^2} e^{\vec{f}^T \vec{x}}, \quad \vec{f} = \sum_i 2\alpha_i t_i \hat{e}_i.$$

$$I = \int_{\mathbb{R}^3} e^{-3t^2} e^{\vec{f}^T \vec{x}} e^{i \frac{\vec{p}^T \vec{x}}{\hbar}} e^{-\frac{1}{2} (\vec{x} - \vec{\theta})^T \Sigma^{-1} (\vec{x} - \vec{\theta})} e^{-\frac{1}{2} \vec{x}^T \underline{\omega} \vec{x}} d^3x$$

$$= \int d^3x \exp\left(-\sum_i t_i^2 + \left(\vec{f}^T + i \vec{p}^T\right) \vec{x} - \vec{x}^T \underline{\omega} \vec{x} - \left(\vec{x}^T \Sigma^{-1} \vec{x} - \vec{x}^T \Sigma^{-1} \vec{\theta} - \vec{\theta}^T \Sigma^{-1} \vec{x} + \vec{\theta}^T \Sigma^{-1} \vec{\theta}\right)\right)$$

$$= \int d^3x \exp\left(-\sum_i t_i^2 - \vec{x}^T (\beta \mathbb{1} + \Sigma^{-1}) \vec{x} + \underbrace{\left(\vec{f}^T + i \vec{p}^T + 2\vec{\theta}^T \Sigma^{-1}\right) \vec{x} - \vec{\theta}^T \Sigma^{-1} \vec{\theta}}_{\vec{b}^T}\right)$$

Let's simplify the exponent: consider the following expression and note that  $\underline{\Delta}$ ,  $\underline{\Sigma}$  are symmetric:

$$\underline{\Delta} (\underline{\Delta}^T \underline{\Delta} = \vec{b}^T \underline{\Delta} \vec{b})$$

$$-(\vec{x} - \vec{\theta})^T \underline{\Delta} (\vec{x} - \vec{\theta}) = -\vec{x}^T \underline{\Delta} \vec{x} + 2\vec{\theta}^T \underline{\Delta} \vec{x} - \vec{\theta}^T \underline{\Delta} \vec{\theta}$$

$$= -\vec{x}^T (\underline{\omega} + \Sigma^{-1}) \vec{x} + \vec{b}^T \vec{x} - \vec{\theta}^T \Sigma^{-1} \vec{\theta}$$

Comparing coefficients yields:

$$\underline{\Delta} = \underline{\omega} + \Sigma^{-1}$$

$$\vec{b}^T \vec{x} = \vec{b}^T \underline{\Delta}^{-1} \underline{\Delta} \vec{x} \Rightarrow \vec{\theta}^T = \frac{1}{2} (\vec{b}^T \underline{\Delta}^{-1})$$

$$\vec{\theta} = \frac{1}{2} (\underline{\Delta}^{-1})^T \vec{b} \quad \text{with} \quad \vec{b} = \vec{f} + i \vec{p} + 2(\Sigma^{-1}) \vec{\theta}$$

$$I = e^{-\sum_i t_i^2} \exp\left(-\vec{\theta}^T \underline{\Delta} \vec{\theta} - \vec{\theta}^T \Sigma^{-1} \vec{\theta}\right) \int d^3x \exp\left\{-\left(\vec{x} - \vec{\theta}\right)^T \underline{\Delta} \left(\vec{x} - \vec{\theta}\right)\right\}$$

$$= Q^{-\sum_i t_i^2} \exp\left(-\vec{\theta}^T \underline{\Delta} \vec{\theta} - \vec{\theta}^T \Sigma^{-1} \vec{\theta}\right) \left(\frac{\pi^3}{|\underline{\Delta}|}\right)^{1/2}$$

Note that  $\vec{\theta}$  contains a  $t_i$  dependency:

$$\vec{\theta}^T \underline{\Delta} \vec{\theta} = \frac{1}{4} \vec{b}^T \underline{\Delta}^{-1} \underline{\Delta} (\underline{\Delta}^{-1})^T \vec{b} = \frac{1}{4} (\underline{\Delta}^{-1} \vec{b})^T \vec{b} = \frac{1}{4} \vec{b}^T (\underline{\Delta}^{-1})^T \vec{b}$$

$$= \sum_i b_i (\underline{\Lambda}^{-1} \underline{b})_i = \sum_{ij} \Lambda_{ij}^{-1} b_i b_j = \sum_{ij} \Lambda_{ij}^{-1} \left( \underbrace{2\alpha_{ii} + i p_i + 2(\sum_k \mu_k)_i}_{c_i} \right) \left( \underbrace{2\alpha_{jj} + c_j}_{c_j} \right)$$

$$= \sum_{ij} \Lambda_{ij}^{-1} (2\alpha_{ii} + c_i) (2\alpha_{jj} + c_j) = \sum_{ij} [4\alpha_i \alpha_j t_i t_j + 2\alpha_i t_i c_j + 2\alpha_j t_j c_i] \Lambda_{ij}^{-1}$$

$$I = \exp \left( - \sum_i t_i^2 + \sum_{ij} [4\alpha_i \alpha_j t_i t_j + 2\alpha_i t_i c_j + 2\alpha_j t_j c_i] \Lambda_{ij}^{-1} \right) \exp \left( - \vec{\mu}^\top \vec{\mu} \right) \left( \frac{\pi^3}{| \Delta |} \right)^{1/2}.$$

Similar to the 1d case, we obtain  $\langle n_1 n_2 n_3 | \Psi(0) \rangle$  as follows:

$$\Psi(\vec{x}, t) = \sum_{n_1} \sum_{n_2} \sum_{n_3} \langle n_1 n_2 n_3 | \Psi(0) \rangle e^{-\frac{i}{\hbar} t E_{n_1 n_2 n_3}} \Psi_{n_1 n_2 n_3}(\vec{x})$$

$$E_{n_1 n_2 n_3} = \hbar \sum_i \omega_i (n_i + \frac{1}{2}), \quad \Psi_{n_1 n_2 n_3}(\vec{x}) = \frac{1}{Z} \prod_{i=1}^3 H_{n_i}(\alpha_i x_i) e^{-\vec{x}^\top \underline{\omega} \vec{x}}$$

$$\langle n_1 n_2 n_3 | \Psi(0) \rangle = \frac{1}{Z} \frac{\partial^{n_1}}{\partial t_1^{n_1}} \frac{\partial^{n_2}}{\partial t_2^{n_2}} \frac{\partial^{n_3}}{\partial t_3^{n_3}} I$$

$$Z = \prod_i \left( \frac{m \omega_i}{\pi \hbar} \right)^{\frac{1}{4}} \frac{1}{\sqrt{2^n n_i!}}, \quad c_i = i p_i + 2(\sum_k \mu_k)_i, \quad \underline{\Delta} = \underline{\omega} + \underline{\omega}^{-1}$$

$$I = \exp \left( - \sum_i t_i^2 + \sum_{ij} [4\alpha_i \alpha_j t_i t_j + 2\alpha_i t_i c_j + 2\alpha_j t_j c_i] \Lambda_{ij}^{-1} \right) \exp \left( - \vec{\mu}^\top \vec{\mu} \right) \left( \frac{\pi^3}{| \Delta |} \right)^{1/2}.$$