EXPLICIT CALCULATION OF THE DYNAMICS
HARMONIC OSCILLATOR IN ONE DIMENSION

$$U = \frac{1}{2} m\omega^2 x^2 \qquad F = -m\omega^2 x$$

We introduce an arbitrary energy scale ϵ

Set $\sigma = \sqrt{\frac{\epsilon}{m\omega^2}}$ so that $\tau = \sqrt{\frac{\epsilon}{m\sigma^2}}\, t = \omega t$

$$\begin{cases} x_{ad}(\tau+\Delta\tau) = x_{ad}(\tau) + v_{ad}(\tau)\Delta\tau - \frac{1}{2} x_{ad}(\tau)\Delta\tau^2 \\ v_{ad}(\tau+\Delta\tau) = v_{ad}(\tau) - \frac{1}{2}\left(x_{ad}(\tau) + x_{ad}(\tau+\Delta\tau)\right)\Delta\tau \end{cases}$$

where "ad" indicates that all quantities are adimensional

$\left(x_{ad} = \frac{x}{\sigma}\right)$ WE DO NOT WRITE "ad" below

$$x(\tau+\Delta\tau) = \left(1 - \frac{\Delta\tau^2}{2}\right) x(\tau) + \Delta\tau\, v(\tau)$$

(we have replaced $x(\tau+\Delta\tau)$)

$$v(\tau+\Delta\tau) = v(\tau) - \frac{\Delta\tau}{2} x(\tau) - \frac{\Delta\tau}{2}\left[\left(1 - \frac{\Delta\tau^2}{2}\right)x(\tau) + \Delta\tau\, v(\tau)\right]$$

$$= -\Delta\tau\left(1 - \frac{\Delta\tau^2}{4}\right)x(\tau) + \left(1 - \frac{\Delta\tau^2}{2}\right)v(\tau)$$

The evolution can be viewed as a dynamical process

$$\begin{pmatrix} x(\tau+\Delta\tau) \\ v(\tau+\Delta\tau) \end{pmatrix} = \begin{pmatrix} 1 - \frac{\Delta\tau^2}{2} & \Delta\tau \\ -\Delta\tau\left(1 - \frac{\Delta\tau^2}{4}\right) & 1 - \frac{\Delta\tau^2}{2} \end{pmatrix} \begin{pmatrix} x(\tau) \\ v(\tau) \end{pmatrix}$$

In matrix form

$$\begin{pmatrix} x(\tau+\Delta\tau) \\ v(\tau+\Delta\tau) \end{pmatrix} = A \begin{pmatrix} x(\tau) \\ v(\tau) \end{pmatrix}$$

Note $\det A = \left(1+\frac{\Delta\tau^2}{2}\right)^2 - \Delta\tau^2\left(1+\frac{\Delta\tau^2}{4}\right) = 1$

The relation det A implies conservation of phase space volume

$$dx(\tau+d\tau)\,dv(\tau+d\tau) = \left|\cancel{\det}\begin{pmatrix} \frac{\partial x(\tau+d\tau)}{\partial x(\tau)} & \frac{\partial v(\tau+d\tau)}{\partial x(\tau)} \\ \frac{\partial x(\tau+d\tau)}{\partial v(\tau)} & \frac{\partial v(\tau+d\tau)}{\partial v(\tau)} \end{pmatrix}\right| \cdot dx(\tau)\,dv(\tau)$$

this is the Jacobian

$$= |\det A|\,dx(\tau)\,dv(\tau)$$
$$= dx(\tau)\,dv(\tau)$$

EXISTENCE OF A CONSERVED HAMILTONIAN

We want to show that there exists a conserved hamiltonian

$$\begin{cases} x(\tau+\Delta\tau) = a\,x(\tau) + b\,v(\tau) \\ v(\tau+\Delta\tau) = c\,x(\tau) + a\,v(\tau) \end{cases} \quad \text{with } \boxed{a^2 - bc = 1}$$

We look ~~for~~ at $H(\tau) = A\,x(\tau)^2 + B\,v(\tau)^2$

We wish to find A, B such that

$$H(\tau) = H(\tau+\Delta\tau) \quad [\text{conservation}]$$

If $H(\tau)$ is conserved, obviously $\lambda H(\tau)$ is conserved for any λ. We can thus fix one of the two constants. Fix $\boxed{B = \frac{1}{2}}$

$$H(\tau) = \frac{1}{2}\, v(\tau)^2 + A\, x(\tau)^2$$

$$\begin{aligned} H(\tau+\Delta\tau) &= \frac{1}{2}\, v(\tau+\Delta\tau)^2 + A\, x(\tau+\Delta\tau)^2 \\ &= \frac{1}{2}\left[c\,x(\tau) + a\,v(\tau)\right]^2 + A\left(a\,x(\tau) + b\,v(\tau)\right)^2 \\ &= \left(\frac{c^2}{2} + Aa^2\right) x(\tau)^2 + \left(\frac{a^2}{2} + Ab^2\right) v(\tau)^2 \\ &\quad + \left(ac + 2Aab\right) x(\tau)\, v(\tau) \end{aligned}$$

If $H(\tau) = H(\tau+\Delta\tau)$, the term $x(\tau)v(\tau)$ should not be present

$$ac + 2Aab = 0 \qquad\qquad A = -\frac{c}{2b}$$

In this case

we use $a^2 - bc = 1$

$$\frac{c^2}{2} + Aa^2 = \frac{c^2}{2} - \frac{c}{2b}(1 + bc) = \cancel{\frac{c^2}{2}} - \frac{c}{2b} - \cancel{\frac{c^2}{2}} = +A$$

$$\frac{a^2}{2} + Ab^2 = \frac{a^2}{2} - \frac{c}{2b}\, b^2 = \frac{a^2}{2} - \frac{bc}{2} = \frac{1}{2}(a^2 - bc) = \frac{1}{2}$$

Therefore

$$H(\tau) = \frac{1}{2}\, v(\tau)^2 - \frac{c}{2b}\, x(\tau)^2 \qquad\qquad \frac{c}{2b} = -\frac{1}{2}\left(1 - \frac{\Delta\tau^2}{4}\right)$$

$$= \frac{1}{2}\, v(\tau)^2 + \frac{1}{2}\left(1 - \frac{\Delta\tau^2}{4}\right) x(\tau)^2$$

We go back to dimensional units

$$\epsilon H(\tau) = \frac{\epsilon}{2}\, v_{ad}^2(\tau) + \frac{1}{2}\left(1 - \frac{\Delta\tau^2}{4}\right) \epsilon\, x_{ad}(\tau)^2$$

Now $$v = \sqrt{\frac{\epsilon}{m}}\, v_{ad}$$

$$x = \sigma X_{ad} = \sqrt{\frac{\epsilon}{m\omega^2}}\, X_{ad} \qquad t = \frac{T}{\omega}$$

It follows

$$\epsilon H(\tau) = \underbrace{\frac{mv^2}{2} + \frac{1}{2} m\omega^2\left(1 - \frac{\omega^2 \Delta t^2}{4}\right) x^2}$$

This quantity is CONSERVED but it is not the Hamiltonian

$H(\tau) \longrightarrow$ Hamiltonian for $\Delta t = 0$

The existence of a conserved Hamiltonian tells us that we are indeed performing a simulation of a statistical mechanics system

BUT: The Hamiltonian is not the correct one.

- M.D. introduces a systematic bias
- M.C <u>DOES</u> NOT introduce a systematic bias

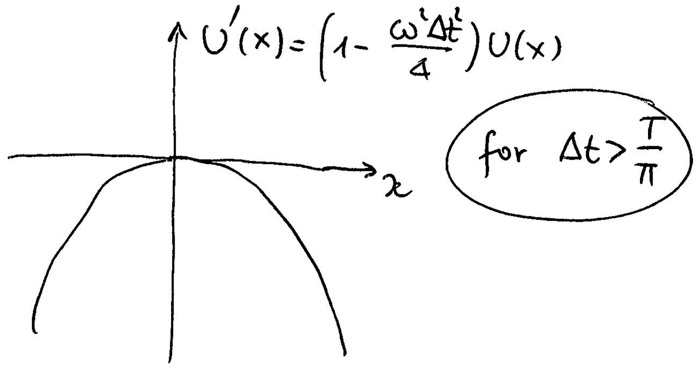
If Δt is small the bias may be SMALL
In principle it can be checked by performing runs with two different value of Δt

However, the existence of a conserved $H(\tau)$ is <u>NOT ENOUGH</u> to guarantee a statistical-mechanics approach.

In the harmonic-oscillator problem note that the potential is not bounded FROM BELOW if

$$1 - \frac{\omega^2 \Delta t^2}{4} < 0 \qquad \Delta t^2 > \frac{4}{\omega^2} \qquad \Delta t > \frac{2}{\omega} = \frac{T}{\pi}$$

If Δt is larger that T/π we have a potential that is not BINDING



If the potential is not bounded from below the dynamics is <u>unstable</u>.

$|x|$ and $|v|$ BOTH increase

IN GENERAL: Δt should be (much) smaller than all "typical times" characterizing the system. Otherwise, the dynamics is unstable.