Week 5 assignment

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Quantum Information and Computation

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Time-dependent Schrödinger equation

Harmonic oscillator, potential moving to the right with $v = \frac{1}{T}$.

$$\hat{H} = \frac{\hat{p}^2}{2} + \frac{\left(\hat{q} - \frac{t}{T}\right)^2}{2} \quad t \in [0, T]$$

Compute

$$|\psi(t)\rangle = U(t)|\psi(0)\rangle$$
$$\langle x|\psi(0)\rangle = \mathcal{N} e^{-\frac{x^2}{2}}$$

Discretizing $T = N_t \Delta t$, with $N_t = 1000$

$$U(t) = e^{-i\int_{t_0}^{t}[\hat{K}+\hat{V}]dt'} \rightarrow e^{-i[\hat{K}+\hat{V}]\Delta t}$$

Split Operator Method

$$e^{-i(\hat{K}+\hat{V})\Delta t} \approx e^{-i\hat{V}\frac{\Delta t}{2}} e^{-i\hat{K}\Delta t} e^{-i\hat{V}\frac{\Delta t}{2}} + \mathcal{O}(\Delta t^3)$$

- When applied $N_t = \frac{T}{\Delta t}$ times, error becomes $N_t \mathcal{O}(\Delta t^3) = \mathcal{O}(\Delta t^2)$
- In momentum basis $\hat{K}$ can be represented as $diag(p_1^2, \dots, p_{N_x}^2)$, the operator above becomes $diag(e^{-ip_1^2 \Delta t}, \dots)$
- With $L = 40$, we choose $N_x = 12000$ for $[-L, L]$. Particle in a box: $p_i \in [-\frac{\pi}{L}, \frac{\pi}{L}]$ with $N_p = N_x$.
- Switching between x, p representation: $\mathcal{F}$
- Time evolution

$$\psi(t + \Delta t) = e^{-\frac{i}{2} V \Delta t} \mathcal{F}^{-1} e^{-iK\Delta t} \mathcal{F} e^{-\frac{i}{2} V \Delta t} \psi(t)$$

Compile: gfortran tdse.f90 -o simulation -llapack -lfftw3 -lfftw3f
Installation: sudo apt-get install -y fftw3-dev

```
do ii = 1, N
        psi(ii) = EXP(-(xlattice(ii)**2d0)/2d0)
    end do
psi = psi / Norm(psi, dxlattice)
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```
function fft(psi) result(psi_p)
    call dfftw_plan_dft_1d(plan, size(psi), psi, psi_p, -1)
    call dfftw_execute_dft(plan, psi, psi_p)
    call dfftw_destroy_plan(plan)
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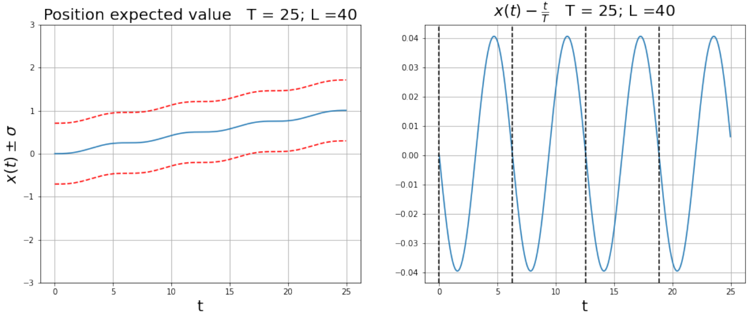
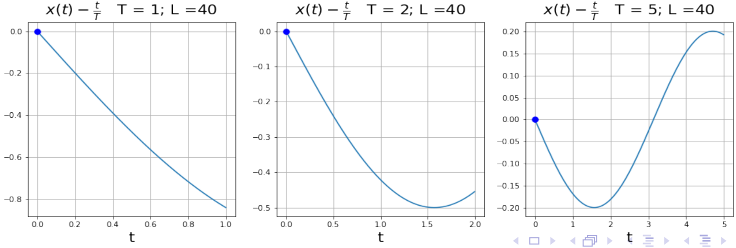
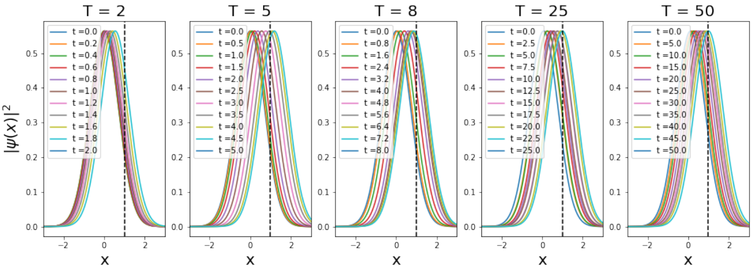
$\hat{q}(t) - \frac{t}{T}$ is the usual position, it should oscillate with period $\frac{2\pi}{\omega}$ ($\omega = 1$).



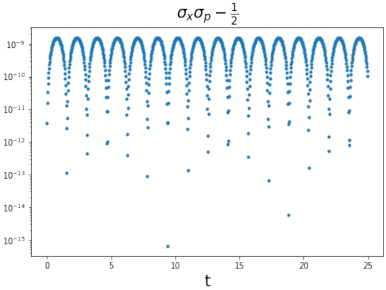
Notice that $\langle x(T) \rangle = 1$, since $\langle x(t) \rangle = vt = \frac{t}{T}$



Only $T = 25, 50$ end with peak at $x = 1$



Heisenberg principle: $\sigma_x \sigma_p \geq \frac{1}{2}$. Ground state of harmonic oscillator falls



in equality case.

$\Delta t^2 \approx 0.6 \cdot 10^{-4}$