PHYS 142/242

Lecture 08: Unitarity and Propagator Trace (Continued)

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Homework reminder

- Half of grade will be from turning in first “draft”
  - Graded on effort and completeness (for all problems)
  - Solution released shortly afterward
- Half of grade will be from turning in corrected solution
  - Graded on effort and correctness (for all problems)
  - ***Note: DO NOT just turn in solutions; CORRECT your own first attempt***
- Report (pdf file) uploaded to Gradescope
- Code (zip file) uploaded to Gradescope
- Assignment 1 correction due Wednesday 8pm!

Path integral → Schrödinger equation

Starting from the path integral $K(x_B, t_B; x_A, t_A) = \int \mathscr{D}x(t) \ \exp\left[\frac{i}{\hbar} S_{\rm cl}[B, A]\right]$,

where $S_{\rm cl}[B, A] = \int_{t_A}^{t_B} \left(\frac{1}{2}m\dot{x}^2 - V(x, t)\right) dt$, and using the fact that the propagator connects states $\psi(x, t)$ and $\psi(x', t')$

$$\psi(x', t') = \int_{-\infty}^{\infty} K(x', t'; x, t)\psi(x, t)dx$$

We can "derive" the Schrödinger equation

$$-\frac{\hbar}{i}\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x, t)\psi(x, t) \equiv \hat{H}\psi(x, t)$$

Schrödinger equation and unitarity

If ψ satisfies SE, its normalization (the total probability) is preserved (*unitarity*)

$$\frac{d}{dt}\left(\int \psi^* \psi dx\right) = 0$$

Equivalent to the fact that the Hamiltonian is a *unitary* operator $\hat{H}^\dagger \hat{H} = 1$

Stationary states

Given a Hamiltonian, there are a set of solutions to the eigenvalue problem

$$\hat{H}\phi_n = E_n\phi_n$$

Solutions are stationary states of definite energy E_n.

They form an *orthonormal and complete* basis

$$\int_{-\infty}^{\infty} \phi_m^*(x)\phi_n(x)dx = \delta_{nm} \quad \text{(orthonormal)} \quad \psi(x,t) = \sum_n c_n e^{-(i/\hbar)E_n t}\phi_n(x) \quad \text{(complete)}$$

Coefficients at any given time $\psi(y, t_1) = f(y)$ can be computed

$$a_n = \int_{-\infty}^{\infty} \phi_n^*(y)f(y)dy$$

Additional relation we found

$$\sum_n \phi_n^*(y)\phi_n(x) = \delta(x-y)$$

Relation to the propagator (1)

Evaluate ψ at a later time t_2 and recall the definition of $a_n = c_n e^{-(i/\hbar)E_n t_1}$

$$\psi(x, t_2) = \sum_{n=1}^{\infty} c_n e^{-(i/\hbar)E_n t_2} \phi_n(x) = \sum_{n=1}^{\infty} a_n e^{-(i/\hbar)E_n(t_2 - t_1)} \phi_n(x)$$

And we have $a_n = \int_{-\infty}^{\infty} \phi_n^*(y) f(y) dy$ where $f(y) = \psi(y, t_1)$

$$\psi(x, t_2) = \sum_{n=1}^{\infty} \left(\int_{-\infty}^{\infty} \phi_n^*(y) f(y) dy \right) e^{-(i/\hbar)E_n(t_2 - t_1)} \phi_n(x)$$

$$= \int_{-\infty}^{\infty} \left(\sum_{n=1}^{\infty} \phi_n^*(y) \phi_n(x) e^{-(i/\hbar)E_n(t_2 - t_1)} \right) f(y) dy$$

Relation to the propagator (2)

What is this equation intuitively?

$$\psi(x,t_2) = \int_{-\infty}^{\infty}\left(\sum_n \phi_n^*(y)\phi_n(x)e^{-(i/\hbar)E_n(t_2-t_1)}\right)\psi(y,t_1)dy$$

If $\psi(x,t) \propto \phi_n(x)$ (just one stationary state), we can time evolve it from t_1 to t_2 by the phase factor

$$\psi(x,t_2) = e^{-(i/\hbar)E_n(t_2-t_1)}\psi(x,t_1)$$

To get it at a different position from y to x, we can apply the Dirac delta function

$$\psi(x,t_1) = \int_{-\infty}^{\infty}\underbrace{\phi_n^*(y)\phi_n(x)}_{\delta(x-y)}\psi(y,t_1)dy$$

This equation picks out the component of ψ along each stationary state ϕ_n, and time evolves it separately (by applying the appropriate phase factor) and shifts to a new position!

Relation to the propagator (3)

Time evolution by projecting onto stationary states

$$\psi(x,t_2) = \int_{-\infty}^{\infty} \left(\sum_n \phi_n^*(y)\phi_n(x)e^{-(i/\hbar)E_n(t_2-t_1)} \right) \psi(y,t_1)dy$$

Time evolution using the propagator

$$\psi(x,t_2) = \int_{-\infty}^{\infty} K(x,t_2;y,t_1)\psi(y,t_1)dy$$

These have to give the same answer so they must be the same!

Propagator and trace

So we have

$$K(x_2, t_2; x_1, t_1) = \begin{cases} \sum_n \phi_n^*(x_2)\phi_n(x_1)e^{-(i/\hbar)E_n(t_2-t_1)} & t_2 > t_1 \\ 0 & t_2 < t_1 \end{cases}$$

We can compute the trace of the propagator just like a matrix. For a matrix K_{ij}, we sum the diagonal components $\mathrm{Tr}(K) = \sum_i K_{ii}$.

Here, we integrate over $x_2 = x_1 = x$. We can also set $t_1 = 0$ and $t_2 = t$.

$$\mathrm{Tr}(K) = \int_{-\infty}^{\infty} dx K(x, t; x, 0) = \sum_n \underbrace{\int_{-\infty}^{\infty} dx \phi_n^*(x)\phi_n(x)}_{1} e^{-(i/\hbar)E_n t} = \sum_n e^{-(i/\hbar)E_n t}$$

Propagator and trace: harmonic oscillator

The Fourier transform of the propagator trace provides the “spectrum” (set of energy eigenvalues)!

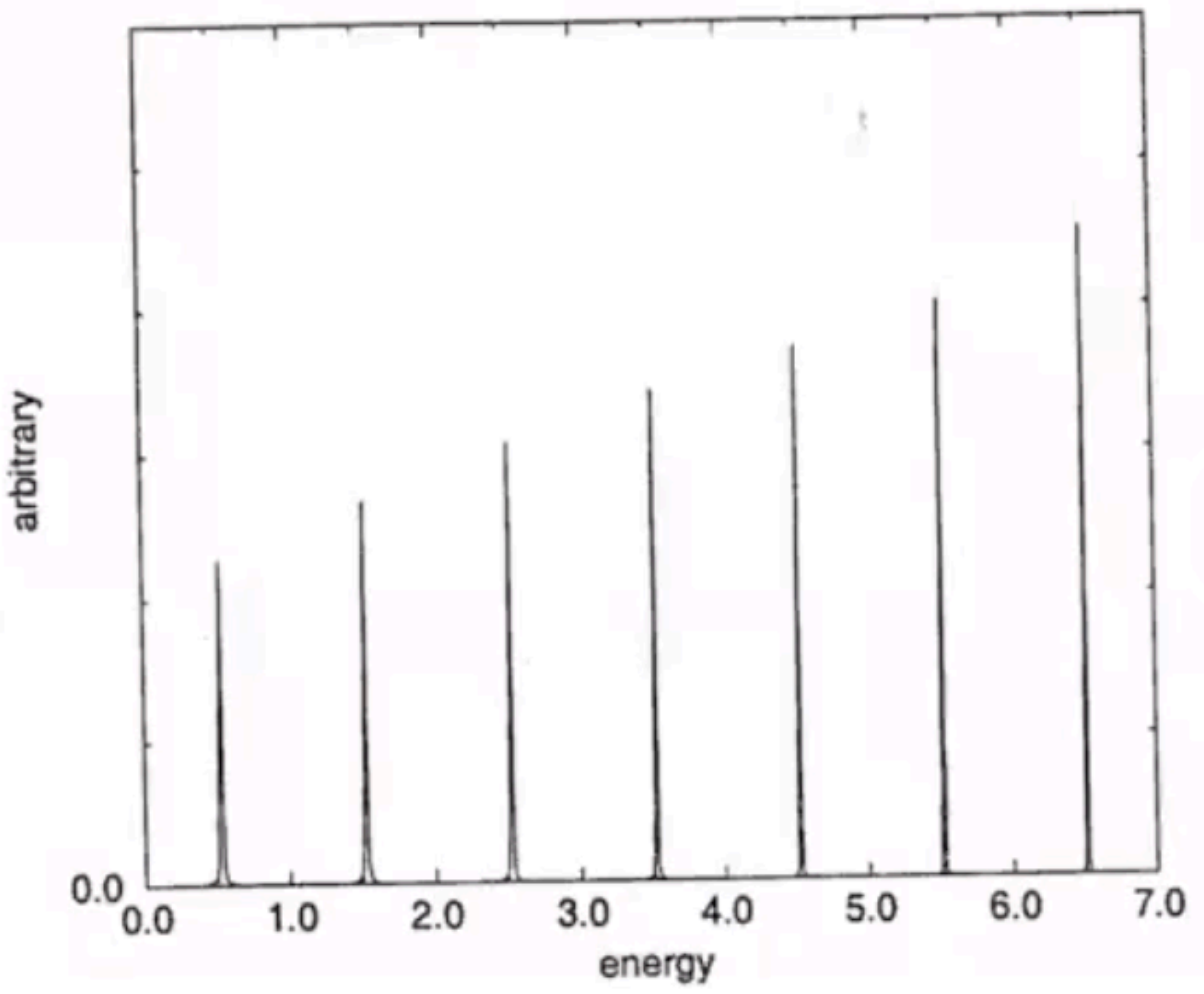
$$\mathrm{Tr}(K) = \sum_n e^{-(i/\hbar)E_n t}$$

For example, for HO, $E_n = \left(n + \frac{1}{2}\right)\hbar\omega$

$$\mathrm{Tr}(K) = \sum_{n=0}^{\infty} e^{-i(n+\frac{1}{2})\omega t} = e^{-i\omega t/2}\sum_{n=0}^{\infty}\left(e^{-i\omega t}\right)^n$$

$$= \frac{e^{-i\omega t/2}}{1 - e^{-i\omega t}} = \frac{1}{e^{i\omega t/2} - e^{-i\omega t/2}}$$

$$= \frac{1}{2i\sin(\omega t/2)}$$



Check for harmonic oscillator

Can explicitly evaluate show that propagator trace for harmonic oscillator gives the same result

$$\mathrm{Tr}(K) = \int_{-\infty}^{\infty} K(x,t;x,0)dx = \int_{-\infty}^{\infty} \left(\frac{m\omega}{2\pi i\hbar \sin \omega t}\right)^{1/2} \exp\left(\frac{im\omega(\cos\omega t - 1)}{\hbar \sin \omega t} x^2\right) dx$$

Recall Gaussian integral: $\int_{-\infty}^{\infty} e^{iax^2} dx = \left(\frac{i\pi}{a}\right)^{1/2}$ and half-angle formula

$1 - \cos(\theta) = 2\sin^2(\theta/2)$

$$\mathrm{Tr}(K) = \left(\frac{m\omega}{2\pi i\hbar \sin\omega t}\right)^{1/2} \left(\frac{i\pi\hbar \sin\omega t}{m\omega(\cos\omega t - 1)}\right)^{1/2} = \left(\frac{1}{2(\cos\omega t - 1)}\right)^{1/2}$$

$$= \frac{1}{2i\sin(\omega t/2)}$$

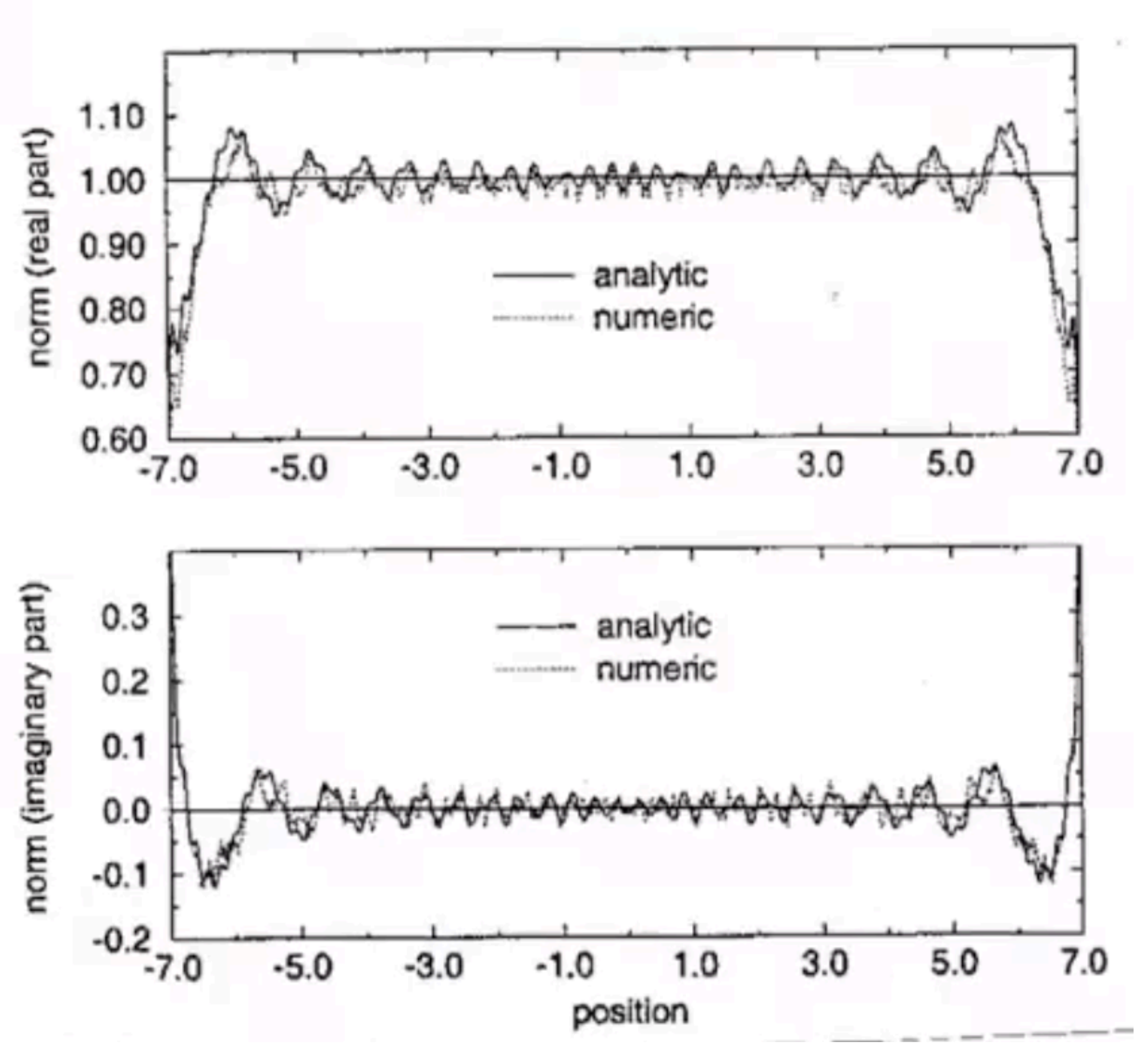
Propagator and unitarity

There is also a normalization condition

$$1 = \int_{-\infty}^{\infty} dx' \langle x' | x \rangle = \int_{-\infty}^{\infty} dx' \delta(x - x') = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dx' dx'' \langle x' | K^\dagger | x'' \rangle \langle x'' | K | x \rangle$$

$$= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dx' dx'' (\langle x'' | K | x' \rangle)^* \langle x'' | K | x \rangle$$

$$= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} K^*(x', t; x'', t) K(x, t; x'', t) dx' dx''$$



Discrete case:

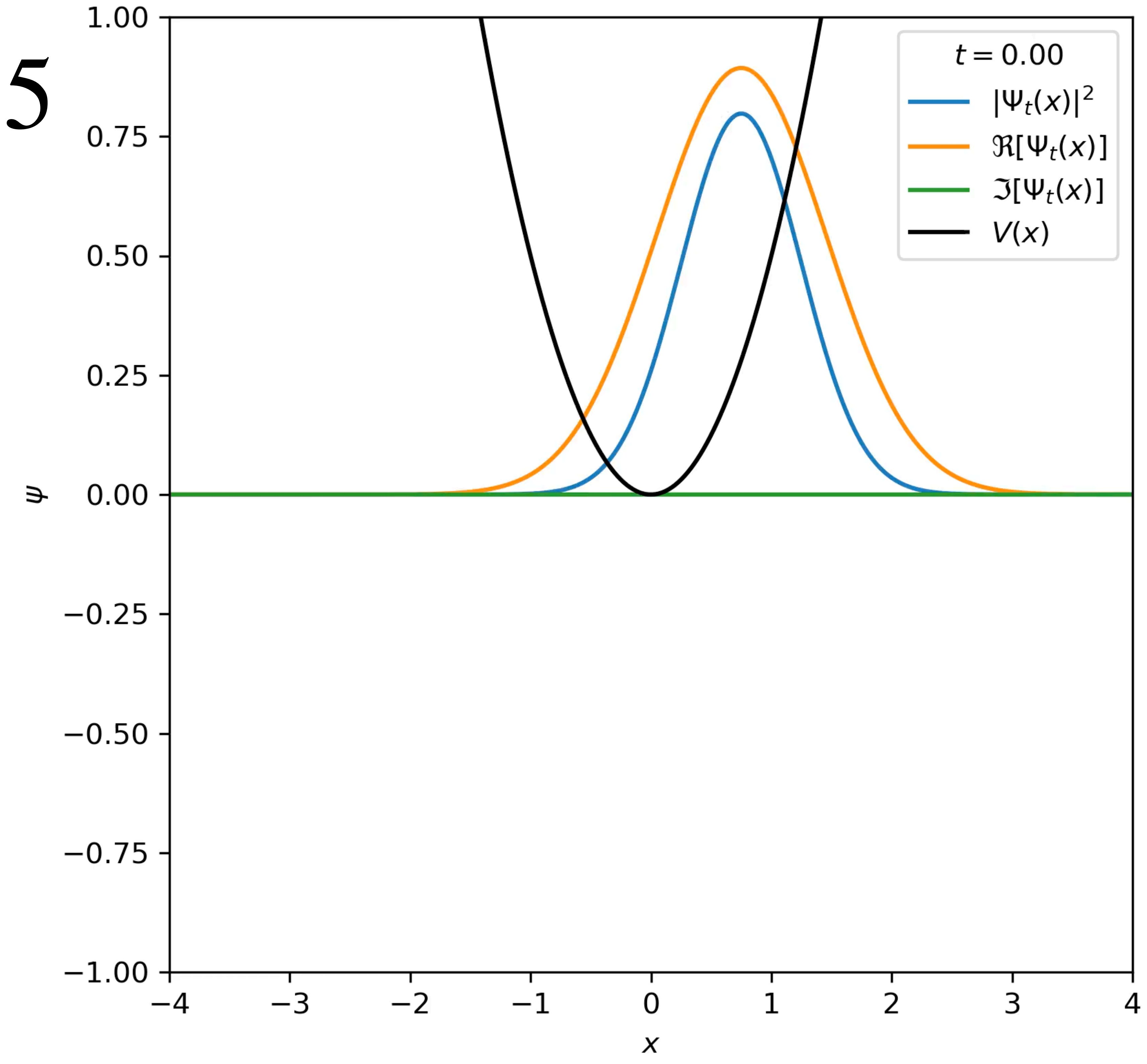
$$1 = \sum_{i=0}^{N_D} \sum_{j=0}^{N_D} (\Delta x)^2 K^*_{ij}(t) K_{ik}(t)$$

Assignment 1: HO

In Assignment 1, we initialize the wave function

$\Psi_0(x) = \left(\frac{\alpha}{\pi}\right)^{1/4} \exp\left(-\frac{\alpha}{2}(x - x_{\text{start}})^2\right)$ where

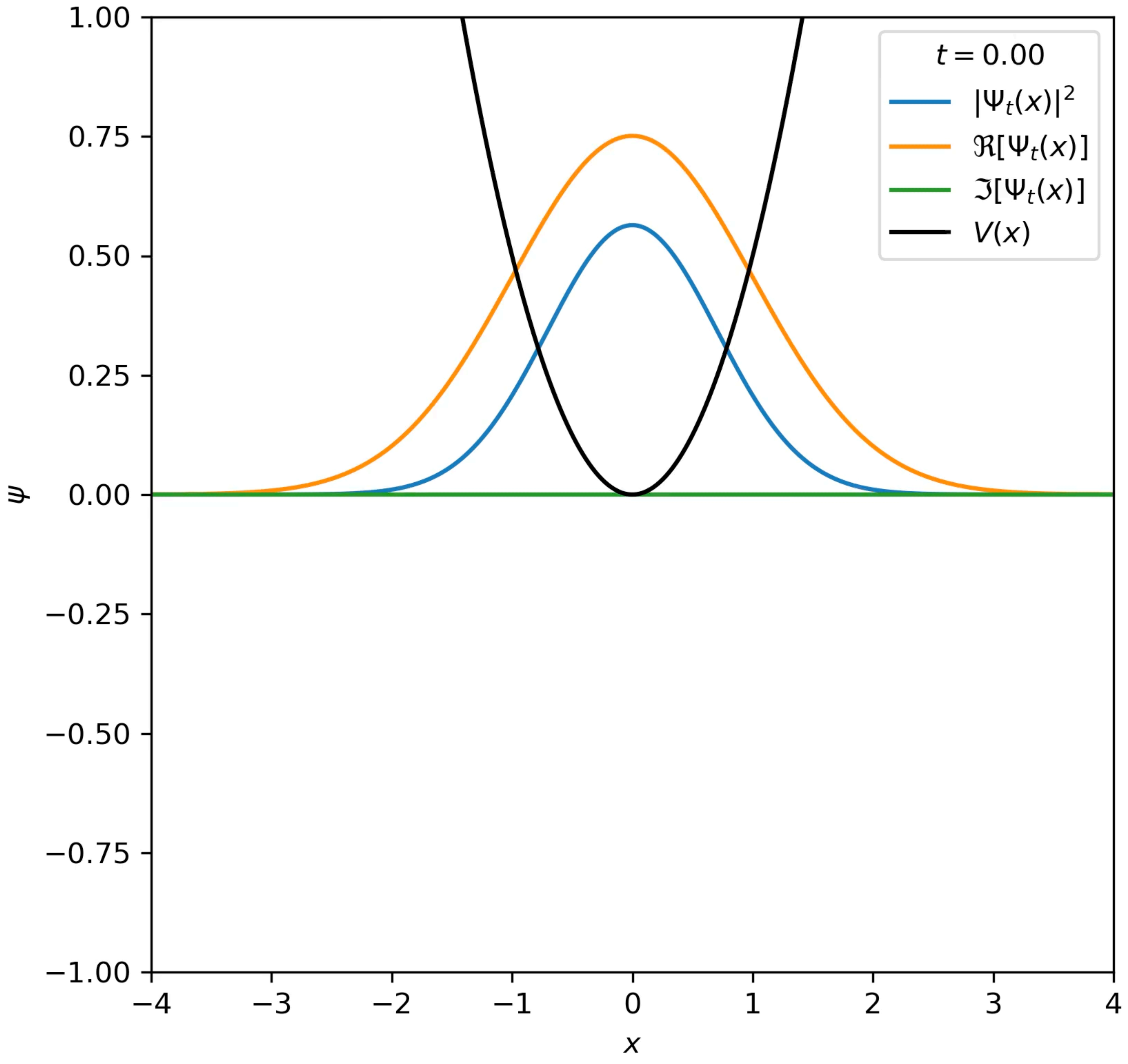
(1) $\alpha = 2,\ x_{\text{start}} = 0.75$



If we set

(2) $\alpha = 1,\ x_{\text{start}} = 0$

Stationary state!



Assignment 1: Propagator

Propagator $K(x, t; x', 0)$ is a matrix. Let's visualize it over time