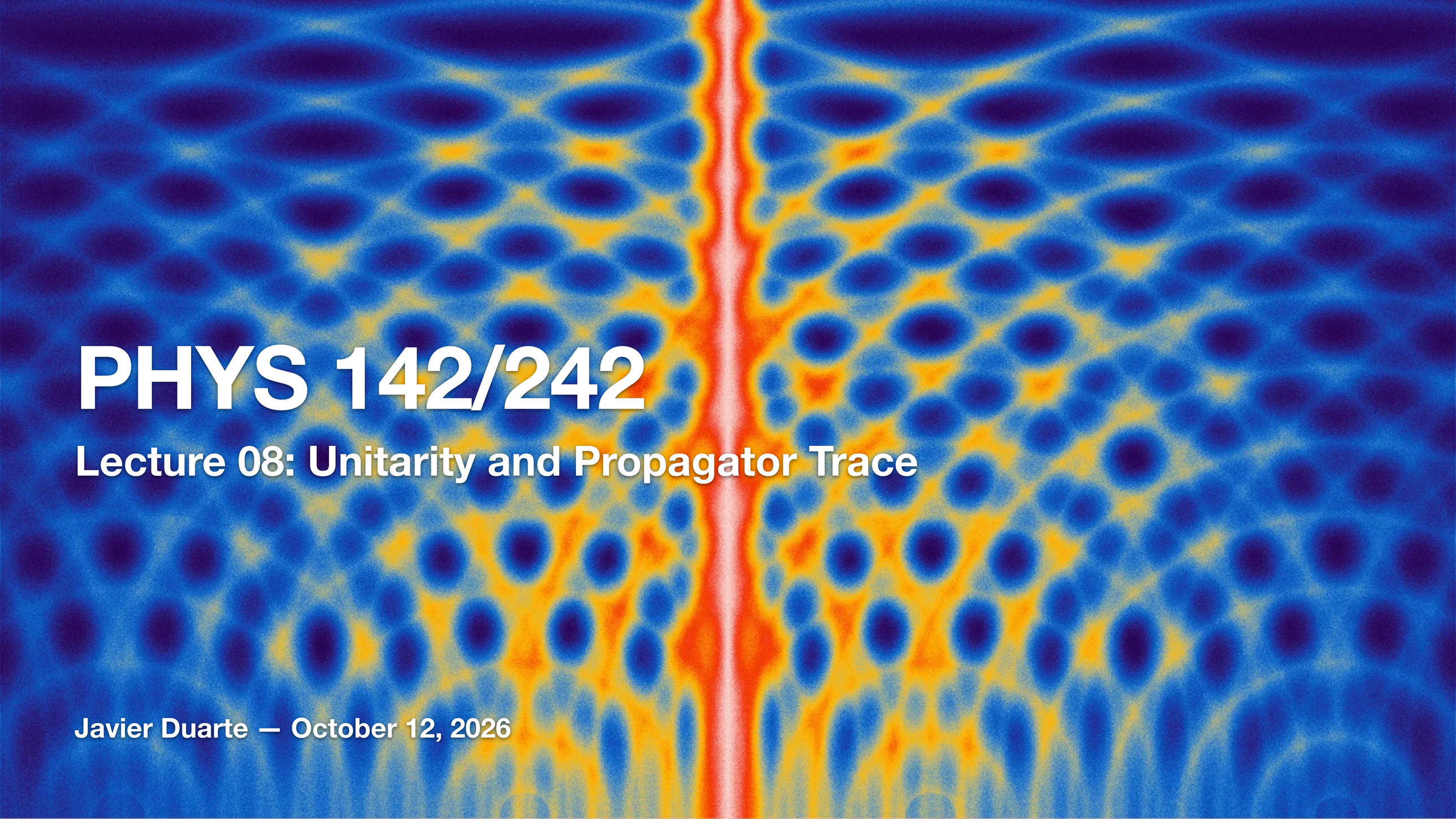


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Lecture 08: Unitarity and Propagator Trace

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Path integral → Schrödinger equation

Last time, we showed that starting from the path integral

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

where $S_{\mathrm{cl}}[B, A] = \int_{t_A}^{t_B} \left(\frac{1}{2} m\dot{x}^2 - V(x, t)\right) dt$, 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

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

Today

Explore the connection between the propagator and the solutions of the Schrödinger equation

Surprising relation: these solutions are encoded in the propagator

Schrödinger equation and unitarity (1)

Defining the Hamiltonian operator $\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V$, then SE is $\hat{H}\psi = \left(-\frac{\hbar}{i}\frac{\partial}{\partial t}\right)\psi$

If ψ satisfies SE, how does the norm $\int |\psi|^2 dx$ change over time?

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

$$= \int \left(\left(\frac{i}{\hbar}\right)\left(-\frac{\hbar^2}{2m}\frac{\partial^2 \psi^*}{\partial x^2} + V\psi^*\right)\psi + \psi^* \left(-\frac{i}{\hbar}\right)\left(-\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + V\psi\right)\right) dx$$

$$= \int \left(\frac{i\hbar}{2m}\left(-\frac{\partial^2 \psi^*}{\partial x^2}\psi + \psi^* \frac{\partial^2 \psi}{\partial x^2}\right) + \frac{iV}{\hbar} \underbrace{\left(\psi^* \psi - \psi^* \psi\right)}_{0} \right) dx$$

Schrödinger equation and unitarity (2)

Now, we can integrate by parts, or equivalently insert

$$\frac{d}{dt}\left(\int \psi^* \psi dx\right) = \int \frac{i\hbar}{2m}\left(-\frac{\partial^2\psi^*}{\partial x^2}\psi + \psi^*\frac{\partial^2\psi}{\partial x^2}\right)dx$$

$$= \int \frac{i\hbar}{2m}\left(-\frac{\partial^2\psi^*}{\partial x^2}\psi - \frac{\partial\psi^*}{\partial x}\frac{\partial\psi}{\partial x} + \frac{\partial\psi^*}{\partial x}\frac{\partial\psi}{\partial x} + \psi^*\frac{\partial^2\psi}{\partial x^2}\right)dx$$

$$= \int \frac{i\hbar}{2m}\frac{\partial}{\partial x}\left(-\frac{\partial\psi^*}{\partial x}\psi + \psi^*\frac{\partial\psi}{\partial x}\right)dx$$

Aside: $j = \frac{\hbar}{2mi}\left(\psi^*\frac{\partial\psi}{\partial x} - \frac{\partial\psi^*}{\partial x}\psi\right)$ is called the *probability current:* $\frac{\partial}{\partial t}(\psi^*\psi) + \frac{\partial j}{\partial x} = 0$

Since this is the integral of a total derivative, we just need to evaluate this $-j$ at $\pm\infty$, but for any well behaved wave function $\psi, \psi^* \to 0$ as $x \to \pm\infty$ so $\frac{d}{dt}\int |\psi|^2 dx = 0$

Schrödinger equation and unitarity (3)

SE implies $\frac{d}{dt}\int |\psi|^2 dx = 0$ so the total probability for the particle to be found somewhere is conserved

If we normalize the wave function to 1 at some time, and it will stay 1 for all time

We call this property of the SE preserving probabilities *unitarity*

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

Stationary states have definite energy

If we can put the particle in a state that doesn't change as we evolve forward in time, we call that a *stationary state* $\phi(x)$

Note there is an overall phase that doesn't affect this quality $\psi(x,t) = e^{-(i/\hbar)Et}\phi(x)$ because $|\psi(x,t)|^2 = |\phi(x)|^2$ so all the probabilities are the same

What is E here? It is the eigenvalue of the Hamiltonian operator $\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V$

$\hat{H}\phi = E\phi$

This E can be interpreted as the energy for the stationary state: stationary states have *definite energy*

Stationary states combine linearly

If we have two different stationary states ϕ_1 and ϕ_2, then their linear combination ψ is also a solution (but not stationary)

$$\psi(x,t) = c_1 e^{(i/\hbar)E_1 t}\phi_1(x) + c_2 e^{(i/\hbar)E_2 t}\phi_2(x)$$

Proof.

$$\begin{aligned}
\hat{H}\psi(x,t) &= c_1 e^{-(i/\hbar)E_1 t}\hat{H}\phi_1(x) + c_2 e^{-(i/\hbar)E_2 t}\hat{H}\phi_2(x) \\
&= c_1 E_1 e^{(i/\hbar)E_1 t}\phi_1(x) + c_2 E_2 e^{-(i/\hbar)E_2 t}\phi_2(x) \\
&= c_1 \left(\frac{\hbar}{i}\frac{\partial}{\partial t}\right)\left(e^{(i/\hbar)E_1 t}\phi_1(x)\right) + c_2 \left(-\frac{\hbar}{i}\frac{\partial}{\partial t}\right)\left(e^{-(i/\hbar)E_2 t}\phi_2(x)\right) \\
&= \left(-\frac{\hbar}{i}\frac{\partial}{\partial t}\right)\psi(x,t)
\end{aligned}$$

Stationary states are orthonormal

Stationary states are *orthonormal*

$$\int_{-\infty}^{\infty} \phi_m^*(x)\phi_n(x)dx = \delta_{nm}$$

Proof. We know $\hat{H}\phi_n = E_n\phi_n$ and $\hat{H}\phi_m = E_m\phi_m$. So we can write

$$E_n \int_{-\infty}^{\infty} \phi_m^*(x)\phi_n(x)dx = \int_{-\infty}^{\infty} \phi_m^*(x)(\hat{H}\phi_n(x))dx$$

and

$$E_m \int_{-\infty}^{\infty} \phi_m^*(x)\phi_n(x)dx = \int_{-\infty}^{\infty} (\hat{H}\phi_m(x))^*\phi_n(x))dx$$

These are the same!

We can subtract the two: $(E_n - E_m)\int_{-\infty}^{\infty} \phi_m^*(x)\phi_n(x)dx = 0$

If $E_n \neq E_m$, the integral must be zero, and if $E_n = E_m$, we already know the integral is 1.

Stationary states are complete

Stationary states are a complete basis.

So any wave function ψ is a linear superposition of stationary states

$$\psi(x,t) = \sum_n c_n e^{-(i/\hbar)E_n t}\phi_n(x)$$

Relation to the propagator (1)

We will compare two ways to time evolve ψ to find a relationship between the stationary states and the propagator

$$\psi(x,t) = \sum_n c_n e^{-(i/\hbar)E_n t}\phi_n(x)$$

In the first way, to calculate the time evolution, we just need to solve for the coefficients of the expansion c_n. Let's do this first at time t_1 then at a later time t_2

$$f(x) = \psi(x,t_1) = \sum_n \underbrace{c_n e^{-(i/\hbar)E_n t_1}}_{a_n}\phi_n(x) = \sum_n a_n\phi_n(x)$$

To find a_m, we can use the orthonormal property of the basis, multiplying by ϕ_m^* and integrating

$$\int_{-\infty}^{\infty}\phi_m^*(x)f(x)dx = \sum_n a_n \underbrace{\int_{-\infty}^{\infty}\phi_m^*(x)\phi_n(x)dx}_{\delta_{nm}} = a_m$$

Relation to the propagator (2)

Now, we can find another useful property, by plugging in a_n that we just solved for

$$f(x) = \psi(x, t_1) = \sum_n a_n \phi_n(x) = \sum_n \left(\int_{-\infty}^{\infty} \phi_n^*(y) f(y) dy \right) \phi_n(x)$$

$$= \int_{-\infty}^{\infty} \left(\sum_n \phi_n^*(y) \phi_n(x) \right) f(y) dy$$

The only way this identity works if this combination is the Dirac delta function

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

Relation to the propagator (3)

We can now evaluate ψ at a later time t_2 and recall the definition of $a_n = c_n e^{-(i/\hbar)E_n t}$

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

But we also found we could found we could compute $a_n = \int_{-\infty}^{\infty} \phi_n^*(y) f(y) dy$ where $f(y) = \psi(y, t_1)$

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

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

Relation to the propagator (4)

So we have

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

But the propagator gives us the same thing!

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

Alternative notation

- Previously we said the propagator can be written

$$K(x_B, t_B; x_A, t_A) = \langle x_B | e^{-i\hat{H}(t_B - t_A)/\hbar} | x_A \rangle,$$

- Unitary time evolution:

$$|\psi(t_B)\rangle = e^{-i\hat{H}(t_B - t_A)/\hbar} |\psi(t_A)\rangle$$

- Applying the propagator (two different bases, but both are just inserting unity!)

$$\langle x_B | \psi(t_B) \rangle = \int \langle x_B | e^{-i\hat{H}(t_B - t_A)/\hbar} | x_A \rangle \langle x_A | \psi(t_A) \rangle dx_A$$

$$\langle x_B | \psi(t_B) \rangle = \sum_n \langle x_B | e^{-i\hat{H}(t_B - t_A)/\hbar} | E_n \rangle \langle E_n | \psi(t_A) \rangle$$

Propagator and trace

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

Compute the trace of the propagator just like a matrix. For matrix K_{ij} it means 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

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

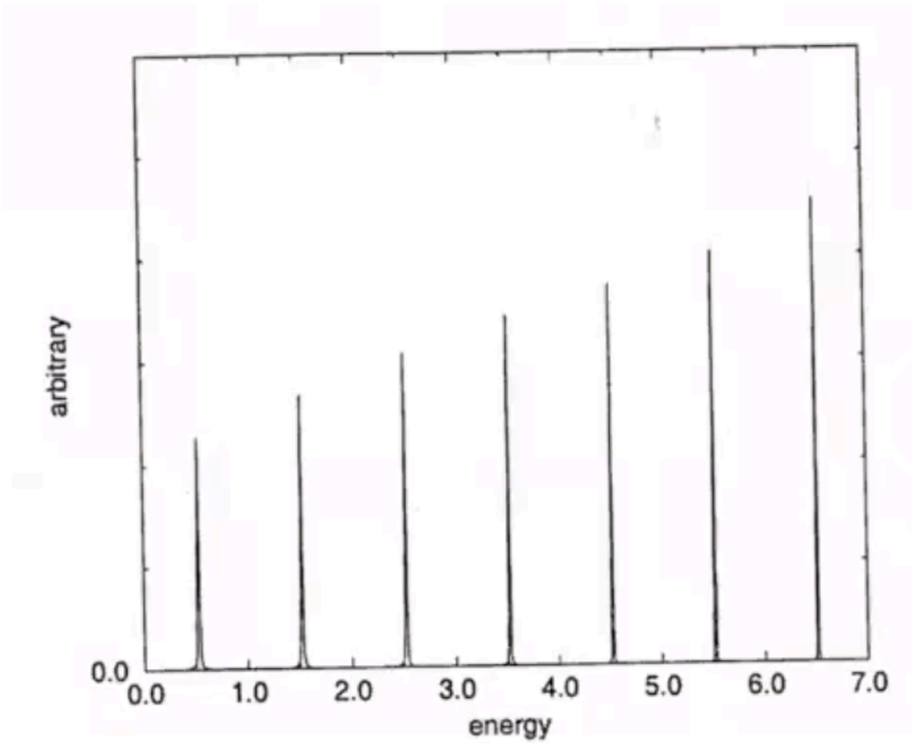
$$\mathrm{Tr}(K) = \sum_n e^{-(i/\hbar)E_n t}$$

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

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

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

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



Bonus exercise for harmonic oscillator

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

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

Hint: Gaussian integral!