E813: Propagator of a Harmonic Oscillator

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The problem:

(1) Find the propogator of a harmonic oscillator of frequency Ω
(2) Take the limit $\Omega \to 0$. What is the meaning of the result?
(3) Derive the partition function $Z = Tr[e^{-\beta \hat{H}}]$ for the harmonic oscillator.
(4) Compare the result of (3) with "classical" sum $Z = \sum_n e^{-\beta E_n}$.
(5) Write an expression for the matrix elements of the equilibrium density operator

$$\rho_\beta(x|x') = \frac{1}{Z}\langle x|e^{-\beta \hat{H}}|x'\rangle$$

The solution:

(1) We will use Van Vleck's approximation which is exact for a harmonic oscillator. First we must calculate the classical action. We know that the classical equation of motion is:

$$x_{cl}(t) = A\sin(\Omega t) + B\cos(\Omega t)$$

Setting the conditions that $x(t=0) = x_0$ and $x(t = t_f) = x_f$ we get:

$$B = x_0$$

$$A = \frac{x_f - x_0\cos(\Omega t_f)}{\sin(\Omega t_f)}$$

The classical Lagrangian is the familiar form:

$$\mathcal{L} = T - V = \frac{1}{2}m\dot{x_{cl}}^2 - \frac{1}{2}m\Omega^2 x_{cl}^2$$

Deriving x_{cl} and plugging into the Lagrangian we get the classical action:

$$\mathcal{A} = \int_0^{t_f} \mathcal{L}dt = \frac{1}{2}m\Omega\left[(A^2 - B^2)\sin(\Omega t_f)\cos(\Omega t_f) - 2AB\sin^2(\Omega t_f)\right]$$

Inserting the values of A and B and after a little algebra we have the classical action:

$$\mathcal{A} = \frac{m\Omega}{2\sin(\Omega t_f)}\left((x_0^2 + x_f^2)\cos(\Omega t_f) - 2x_0x_f\right)$$

To complete the Van Vleck calculation we need the prefactor:

$$\frac{\partial^2\mathcal{A}}{\partial x_f \partial x_0} = \frac{m\Omega}{\sin(\Omega t_f)}$$

Giving us the propagator as required (substituting $x = x_f, t = t_f$ for clarity) :

$$U(x|x_0) = \left(\frac{m\Omega}{2\pi i\sin(\Omega t)}\right)^{\frac{1}{2}} e^{i\frac{m\Omega}{2\sin(\Omega t)}\left((x_0^2+x^2)\cos(\Omega t) - 2x_0x\right)}$$

(2) Taking the limit $\Omega \to 0$ means that we replace:

$$\frac{\Omega}{\sin(\Omega t)} \to \frac{1}{t}$$

$$\cos(\Omega t) \to 1$$

This gives us the propagator for a free particle, as we would expect:

$$U(x|x_0)_{\Omega\to 0} = \left(\frac{m}{2\pi i t}\right)^{\frac{1}{2}} e^{i\frac{m}{2t}(x-x_0)^2}$$

(3) We can calculate the partition function as

$$Z = \int \langle x|e^{-\beta\hat{H}}|x\rangle dx$$

By comparing with the propagator in position representation:

$$U(x|x_0) = \langle x|e^{-\frac{i}{\hbar}t\hat{H}}|x_0\rangle$$

we see that we already have the solution, once we perform a "Wick Rotation" which is nothing but

$$t = -i\hbar\beta$$

meaning that the temperature is replaced by imaginary time. The full Trotter decomposition can now be done similarly to the derivation in the lecture notes, (this is the method used in quantum monte-carlo simulations), but it is not required of us since for our purposes we can simply use the result from section (1) to get

$$Z = \int_{-\infty}^{\infty} \left(\frac{m\Omega}{2\pi\hbar\sinh(\Omega\beta\hbar)}\right)^{\frac{1}{2}} e^{\frac{m\Omega}{2\sinh(\Omega\beta\hbar)}\left(2x^2\cosh(\Omega\beta\hbar)-2x^2\right)}dx$$

This integral seems monstrous at a glance, but is in fact a simple Gaussian integral, and after a little math we get the result

$$Z = \frac{1}{2\sinh(\frac{\Omega\beta\hbar}{2})}$$

(4) We check the result of section (3) by comparing it with the explicit calculation

$$Z = \sum_{n=0}^{\infty} e^{-\beta\hbar\Omega(n+\frac{1}{2})} = e^{\frac{-\beta\hbar\Omega}{2}}\frac{1}{1-e^{-\beta\hbar\Omega}} = \frac{1}{2\sinh(\frac{\Omega\beta\hbar}{2})}$$

(5) Since we have Z and the expression $\langle x|e^{-\beta\hat{H}}|x'\rangle$ can be calculated directly using the same technique as in section (3) we get:

$$\rho_\beta(x|x') = \frac{1}{Z}\left(\frac{m\Omega}{2\pi\hbar\sinh(\Omega\beta\hbar)}\right)^{\frac{1}{2}} e^{\frac{-m\Omega}{2\hbar\sinh(\Omega\beta\hbar)}\left((x+x')^2\cosh(\Omega\beta\hbar)-2xx'\right)}$$