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Contents

Disclaimer: This document is a concise guide for the lectures of the course Introduction to Path Integrals given in the I Escola Avançada de Física Teórica, São Carlos, July 2016. It is not suppose to substitute any text book and neither the discussions of the physical content in the lectures. The purpose of these notes it to help the students to go through the mathematical steps. There are many high quality books on the subject. We suggest, for example, *Condensed Matter Field Theory* by Altland & Simons, and *Quantum Field Theory of Many-Body System* by Wen.

I. THE TIME EVOLUTION OPERATOR

Given a initial quantum state $\left|\psi\left(t_i\right)\right\rangle$, we are interested in how the system state evolves as time goes on. This is given by the time evolution operator defined from

$$\left|\psi\left(t_f\right)\right\rangle \equiv \hat{U}\left(t_f, t_i\right)\left|\psi\left(t_i\right)\right\rangle, \text{ where } t_f > t_i, \tag{1}$$

and with the constraint that $\hat{U}\left(t_i, t_i\right) = \mathbb{I}$. Some properties are straightforward: the composition property $\hat{U}\left(t_3, t_2\right)\hat{U}\left(t_2, t_1\right) = \hat{U}\left(t_3, t_1\right)$ (with $t_3 \geq t_2 \geq t_1$), and unitarity $\hat{U}\left(t_2, t_1\right)\hat{U}^{\dagger}\left(t_2, t_1\right) = \mathbb{I}$, which comes from probability conservation $\langle\psi|\psi\rangle = 1$ for any t.

The time evolution operator can be determined from the Schrödinger equation: $i\hbar\frac{\partial}{\partial t}|\psi\rangle = H|\psi\rangle$, $\Rightarrow$ $i\hbar\frac{\partial}{\partial t}\hat{U}\left(t, t_0\right)\left|\psi_0\right\rangle = \hat{H}\hat{U}\left(t, t_0\right)\left|\psi_0\right\rangle$, for any $\left|\psi_0\right\rangle$. Thus,

$$i\hbar\frac{\partial}{\partial t}\hat{U} = \hat{H}\hat{U}. \tag{2}$$

It is interesting to recall that for time-independent $\hat{H}$, then $\hat{U}\left(t, t_0\right) = e^{\frac{1}{i\hbar}\left(t-t_0\right)\hat{H}}\Theta\left(t-t_0\right)$, where $\Theta\left(x\right)$ is the Heaviside function [1]. In this case, notice that $\hat{U}\left(t, t_0\right) \equiv \hat{U}\left(t-t_0\right)$ as a consequence of energy conservation. In addition, for an infinitesimal time evolution, then $\hat{U}\left(t+\mathrm{d}t, t\right) = \mathbb{I} + \frac{1}{i\hbar}\mathrm{d}t\hat{H} = e^{\frac{1}{i\hbar}\mathrm{d}t\hat{H}(t)}$, regardless whether the Hamiltonian is time independent or not.

II. THE PROPAGATOR

Mathematically, the propagator$G$ is simply defined as a matrix element of the time evolution operator:

$$i\hbar G\left(x_f, t_f, x_i, t_i\right) \equiv \left\langle x_f \left|\hat{U}\left(t_f, t_i\right)\right| x_i\right\rangle. \tag{3}$$

The first thing we have to notice is that the propagator depends on the representation, i.e., it depends on the basis we are considering. For the case of a $\hat{H}$ describing a particle moving in some external potential and $|x\rangle$ denoting the physical state in which a particle is located at position x, then $|i\hbar G|^2$ represents the probability density of this particle going from $\left(x_i, t_i\right) \rightarrow \left(x_f, t_f\right)$. Notice nothing is said about the initial state of the particle.

Defined in this way, we can compute the particle wavefunction $\psi\left(x, t\right)$ at time t given that it is known at a previous time t_0:

$$\begin{aligned}\psi\left(x, t\right) = \langle x|\psi\left(t\right)\rangle = \left\langle x\left|\hat{U}(t, t_0)\right|\psi\left(t_0\right)\right\rangle = \int\left\langle x\left|\hat{U}(t, t_0)\right|x_0\right\rangle\left\langle x_0|\psi\left(t_0\right)\right\rangle\mathrm{d}x_0 \\ = i\hbar\int G\left(x, t, x_0, t_0\right)\psi\left(x_0, t_0\right)\mathrm{d}x_0,\end{aligned} \tag{4}$$

where we have used that $\mathbb{I} = \int\mathrm{d}x_0\left|x_0\right\rangle\left\langle x_0\right|$. In this way, the propagator G can also be viewed as the Green's function of the Schrödinger equation.

A. Detour1: The free-particle propagator via Schrödinger equation

For a free particle ($\hat{H} = \frac{1}{2m}\hat{p}^2$), the Schrödinger equation simply gives us $\hat{U} = e^{\frac{1}{i2m\hbar}\left(t-t_0\right)\hat{p}^2}$. Thus, in the momentum representation, we have $\left\langle p\left|\hat{U}\right|p_0\right\rangle = \delta\left(p-p_0\right)e^{\frac{1}{i2m\hbar}\left(t-t_0\right)p^2}$, where $\hat{p}\left|p_0\right\rangle = p_0\left|p_0\right\rangle$.

If we are interested in the position representation, we use that $\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}}e^{i\frac{px}{\hbar}}$

$$i\hbar G = \left\langle x\left|\hat{U}\right|x_0\right\rangle = \int\mathrm{d}p\mathrm{d}p_0\langle x|p\rangle\left\langle p\left|\hat{U}\right|p_0\right\rangle\left\langle x_0|p_0\right\rangle = \frac{1}{2\pi\hbar}\int\mathrm{d}pe^{\frac{1}{i\hbar}\left(\left(\frac{t-t_0}{2m}\right)p^2-\left(x-x_0\right)p\right)} = \sqrt{\frac{m}{2\pi i\hbar\left(t-t_0\right)}}e^{\frac{i}{\hbar}S_{\mathrm{cl}}}, \tag{5}$$

where $S_{\mathrm{cl}}\left(x, t, x_0, t_0\right) = \frac{m\left(x-x_0\right)^2}{2\left(t-t_0\right)}$ is the classical action of a free particle (which comes from the path of constant velocity). Here, we have used the result $\int_{-\infty}^{\infty}e^{-i\left(ax^2+bx\right)}\mathrm{d}x = \sqrt{\frac{\pi}{ia}}e^{i\frac{b^2}{4a}}$ (see Sec. IX). Notice that from translational and time invariance of $\hat{H}$, then $G\left(x, t, x_0, t_0\right) = G\left(x-x_0, t-t_0\right)$.

B. Detour2: The propagator in the frequency space

Consider the propagator in the energy representation (with $\hat{H}$ being time-independent)

$$i\hbar G_E\left(\phi_2,t_2,\phi_1,t_1\right)\equiv i\hbar G_E\left(\phi_2,\phi_1,t_2-t_1\right)=\left\langle \phi_2\left|\hat{U}\left(t_2,t_1\right)\right|\phi_1\right\rangle=\delta_{\phi_2,\phi_1}e^{\frac{1}{i\hbar}E_2\left(t_2-t_1\right)}, \tag{6}$$

where $\hat{H}\left|\phi_i\right\rangle=E_i\left|\phi_i\right\rangle$. Defining the Fourier transform

$$\begin{aligned}\tilde{G}_E\left(\phi_2,\phi_1,\omega\right)&=\int G_E\left(\phi_2,\phi_1,t\right)e^{i\omega t}\mathrm{d}t=\frac{\delta_{\phi_2,\phi_1}}{i\hbar}\int_0^\infty e^{\frac{1}{i\hbar}E_2t+i\omega t}\mathrm{d}t\\&=\frac{\delta_{\phi_2,\phi_1}}{i\hbar\left(\frac{1}{i\hbar}E_2+i\omega\right)}\left.e^{\frac{1}{i\hbar}E_2t+i\omega t}\right|_{t=0}^{\infty}=\frac{-\delta_{\phi_2,\phi_1}}{E_2-\hbar\left(\omega+i\eta\right)}=\frac{\delta_{\phi_2,\phi_1}}{\hbar\omega-\left(E_2-i0^+\right)}.\end{aligned}$$

Here, we replaced ω with a complex number $\omega=\omega+i\eta$ and take the limit $\eta\to0^+$ in order to converge the integral: $\lim_{t\to\infty}e^{\frac{1}{i\hbar}E_2t+i\omega t}=0$. For short, we write $\hbar\eta=0^+$.

We can now use this result in order to compute the propagator in the frequency space

$$G\left(x,x_0,\omega\right)=\frac{1}{i\hbar}\left\langle x\left|\hat{U}\right|x_0\right\rangle=\sum_{\phi,\phi'}\left\langle x|\phi\right\rangle\tilde{G}_E\left(\phi,\phi',\omega\right)\left\langle\phi'|x_0\right\rangle=\sum_{\phi}\frac{\left\langle x|\phi\right\rangle\left\langle\phi|x_0\right\rangle}{\hbar\omega-\left(E_\phi-i0^+\right)}.$$

This is an interesting result. From the structure of the poles of $G\left(x,x_0,\omega\right)$, we can obtain the spectrum of $\hat{H}$.

Finally, if we want to recover the G_E from $\tilde{G}_E$, we have to inverse-Fourier transform

$$G_E\left(\phi_2,\phi_1,t\right)=\int\frac{\mathrm{d}\omega}{2\pi}\frac{\delta_{\phi_2,\phi_1}e^{-i\omega t}}{\hbar\omega-\left(E_2-i0^+\right)}=2\pi i\sum_{\text{Residues}}\frac{1}{2\pi}\left(\frac{\delta_{\phi_2,\phi_1}e^{-i\omega t}}{\hbar\omega-\left(E_2-i0^+\right)}\right).$$

For $t>0$, we choose the contour in the lower half of the complex plane because $e^{-i\omega t}\propto e^{t\mathrm{Im}(\omega)}$ and $\mathrm{Im}\left(\omega\right)<0$. In this case, there is a pole inside the contour which is at $\hbar\omega=E_2-i0^+$ In addition, there is a global minus signal because the contour is clockwise. For $t<0$, we need to choose the upper half-plane. However, in this case, there is no pole inside the contour. Thus, $G_E=0$ for $t<0$. Finally,

$$G_E\left(\phi_2,\phi_1,t\right)=-\frac{i}{\hbar}\times\delta_{\phi_2,\phi_1}e^{-i\left(\frac{E_2-i0^+}{\hbar}\right)t}\Theta\left(t\right)=\frac{1}{i\hbar}\delta_{\phi_2,\phi_1}e^{\frac{1}{i\hbar}E_2t}\Theta\left(t\right),$$

which recovers the result (6).

III. PATH INTEGRAL REPRESENTATION OF A PARTICLE PROPAGATOR

For simplicity, let us consider the Hamiltonian $\hat{H}=\frac{1}{2m}\hat{p}^2+\hat{V}\left(x,t\right)$ describing a single particle propagating in 1D under the influence of an external potential. As will become clear in the following derivation of the path integral representation, it is straightforward to generalize it for a general Hermitean Hamiltonian.

The propagator is obtained from

$$i\hbar G(x_ft_f,x_i,t_i)=\left\langle x_f\left|\hat{U}\left(t_f,t_i\right)\right|x_i\right\rangle,$$

and $\hat{U}$ can be obtained from solving the Schrödinger equation (2). An alternative approach for this usual quantum mechanics prescription is the path integral formulation of the quantum mechanics. Instead of solving the Schrödinger equation, we evolve the system through N intermediate time steps, each of which are of duration $\Delta t=\frac{t_f-t_i}{N}$, i.e.,

$$\hat{U}(t_f,t_i)=\hat{U}(t_N,t_{N-1})\ldots\hat{U}(t_2,t_1)\hat{U}(t_1,t_0), \tag{7}$$

where $t_k=t_0+k\Delta t$, $t_0=t_i$, and $t_N=t_f$.

Let us consider the case of $N=2$. Thus,

$$\begin{aligned}i\hbar G\left(2,0\right)&=\left\langle x_f\left|\hat{U}\left(t_2,t_1\right)\hat{U}\left(t_1,t_0\right)\right|x_i\right\rangle=\int\mathrm{d}x_1\left\langle x_f\left|\hat{U}\left(t_2,t_1\right)\right|x_1\right\rangle\left\langle x_1\left|\hat{U}\left(t_1,t_0\right)\right|x_i\right\rangle\\&=\int\mathrm{d}x_1 i\hbar G\left(2,1\right)\times i\hbar G\left(1,0\right).\end{aligned} \tag{8}$$

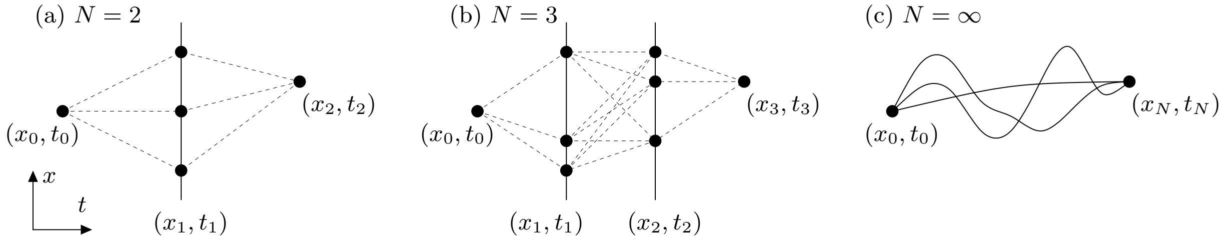

Figure 1: Schematic visualization of the superposition principle in quantum mechanics.

This highlights the superposition principle in Quantum Mechanics. Recalling that $G(f,i)$ is the amplitude probability density of the system going from $i \to f$, then the right-hand side of (8) tells us that the system goes from the initial configuration (x_i,t_i) to the final one (x_f,t_f) via all possible intermediate configurations (x_1,t_1) in between (see panel (a) of Fig. 1). This is just like the double-slit experiment (although here we are considering infinitely many slits) and it is a simple consequence of the wavelike character of the quantum particle. In the schematic representation of Fig. 1, the dashed lines are representative trajectories since no such concept exists in quantum (or wave) mechanics. When increasing the number of intermediate steps [see panel (b)], it is like we were inquiring more often the particle current position. In the extreme limit of $N \to \infty$ [see panel (c)], the particle position is inquired at all time instants and the concept of a classical trajectory arises. The superposition principle in quantum mechanics simply states that all these possible paths interfere with each other.

It is now our task to quantify how these paths interfere with each other. From (7), we have that

$$\begin{aligned} i\hbar G(x_N t_N, x_0, t_0) &= \lim_{N\to\infty} \left\langle x_N \left| \hat{U}(t_N,t_{N-1}) \dots \hat{U}(t_2,t_1)\hat{U}(t_1,t_0) \right| x_0 \right\rangle \\ &= \lim_{N\to\infty} \int \dots \int \mathrm{d}x_1 \dots \mathrm{d}x_{N-1} \left\langle x_N \left| \hat{U}(t_N,t_{N-1}) \right| x_{N-1} \right\rangle \dots \left\langle x_2 \left| \hat{U}(t_2,t_1) \right| x_1 \right\rangle \left\langle x_1 \left| \hat{U}(t_1,t_0) \right| x_0 \right\rangle, \end{aligned}$$

where we have inserted $N-1$ resolutions $\mathbb{I} = \int \mathrm{d}x_k \left| x_k \right\rangle \left\langle x_k \right|$. Let us take a closer look in each of these terms

$$\left\langle x_{k+1} \left| \hat{U}(t_{k+1},t_k) \right| x_k \right\rangle = \left\langle x_{k+1} \left| \hat{U}(t_k+\Delta t,t_k) \right| x_k \right\rangle = \left\langle x_{k+1} \left| e^{\frac{1}{i\hbar}\Delta t \hat{H}(t_k)} \right| x_k \right\rangle.$$

(Although the last passage is valid only in the limit $\Delta t \to 0$, it is also valid for any finite interval Δt as long as $\hat{H}$ is time independent.) Now, we have to compute $\left\langle x_{k+1} \left| e^{\frac{1}{i\hbar}\Delta t\left(\hat{T}+\hat{V}(x,t_k)\right)} \right| x_k \right\rangle$. In general, this is not a simple task because $\hat{T} = \frac{1}{2m}\hat{p}^2$ and $\hat{V}$ do not commute with each other. However, a curious formula exists:

$$e^{\epsilon\left(\hat{X}+\hat{Y}\right)} = e^{\epsilon\hat{X}} e^{\epsilon\hat{Y}} e^{-\frac{1}{2}\epsilon^2[\hat{X},\hat{Y}]} e^{-\frac{1}{3!}\epsilon^3\left(2[\hat{Y},[\hat{X},\hat{Y}]]+[\hat{X},[\hat{X},\hat{Y}]]\right)} \dots.$$

This is the Zassenhaus formula which is related to the more familiar Baker-Campbell-Hausdorff formula [2]. Therefore, we have that $\lim_{\Delta t\to 0} e^{\frac{1}{i\hbar}\Delta t\left(\hat{T}+\hat{V}\right)} = e^{\frac{1}{i\hbar}\Delta t\hat{T}} e^{\frac{1}{i\hbar}\Delta t\hat{V}}$. Basically, the non-commutativity becomes *irrelevant* in the short-time limit [3]. Thus,

$$\begin{aligned} \left\langle x_{k+1} \left| e^{\frac{1}{i\hbar}\Delta t\hat{H}} \right| x_k \right\rangle &= \left\langle x_{k+1} \left| e^{\frac{1}{i\hbar}\Delta t\hat{T}} e^{\frac{1}{i\hbar}\Delta t\hat{V}} \right| x_k \right\rangle = \left\langle x_{k+1} \left| e^{\frac{1}{i\hbar}\Delta t\hat{T}} \right| x_k \right\rangle e^{\frac{1}{i\hbar}\Delta t V(x_k,t_k)} \\ &= \int \mathrm{d}p_k \left\langle x_{k+1} \left| e^{\frac{1}{i\hbar}\Delta t\hat{T}} \right| p_k \right\rangle \left\langle p_k | x_k \right\rangle e^{\frac{1}{i\hbar}\Delta t V(x_k,t_k)} = \int \mathrm{d}p_k \left\langle x_{k+1} | p_k \right\rangle \left\langle p_k | x_k \right\rangle e^{\frac{1}{i\hbar}\Delta t(T(p_k)+V(x_k,t_k))} \\ &= \frac{1}{2\pi\hbar} \int \mathrm{d}p_k e^{-\frac{p_k x_{k+1}}{i\hbar}} e^{\frac{p_k x_k}{i\hbar}} e^{\frac{1}{i\hbar}\Delta t H(p_k,x_k,t_k)} = \frac{1}{2\pi\hbar} \int \mathrm{d}p_k e^{\frac{1}{i\hbar}\Delta t\left[-\left(\frac{x_{k+1}-x_k}{\Delta t}\right)p_k + H(p_k,x_k,t_k)\right]}, \end{aligned}$$

where $H(p_k,x_k) = T(p_k) + V(x_k,t_k)$. It is important to notice that this quantity is *not* an operator, but a scalar.

Collecting all the terms and defining $\dot{x}_k = \left(\frac{x_{k+1}-x_k}{\Delta t}\right)$, we find that

$$\begin{aligned} i\hbar G &= \lim_{N\to\infty} \int \prod_{k=1}^{N-1} \mathrm{d}x_k \prod_{l=0}^{N-1} \frac{\mathrm{d}p_l}{2\pi\hbar} \exp\left[\frac{i}{\hbar}\Delta t \sum_{\ell=0}^{N-1} \left(\dot{x}_\ell p_\ell - H\left(p_\ell, x_\ell, t_\ell\right)\right)\right] \\ &= \int \mathcal{D}\left[q\left(t\right)\right] \exp\left[\frac{i}{\hbar} \int_{t_i}^{t_f} \mathrm{d}t \left(\dot{x}\left(t\right) p\left(t\right) - H\left(p,x,t\right)\right)\right]. \end{aligned} \tag{9}$$

Here, we denote by $\mathcal{D}\left[q\left(t\right)\right]=\lim_{N\to\infty}\prod_{k=1}^{N-1}\mathrm{d}x_k\prod_{l=0}^{N-1}\frac{\mathrm{d}p_l}{2\pi\hbar}$ the functional integral over the phase space. The representation of the propagator in (9) is called the phase space representation of the propagator path integral. Notice the functional $\int_{t_i}^{t_f}\mathrm{d}t\left(\dot{x}\left(t\right)p\left(t\right)-H\left(p,x,t\right)\right)$ has the appealing look of an action. But recall that $\dot{x}$ has no relation with p since they are unrelated dummy variables.

Since $T\left(p_k\right)=\frac{1}{2m}p_k^2$, we can perform a Gaussian integration over the momentum variables: $\int\mathrm{d}p_k e^{\frac{i}{\hbar}\Delta t\left[\dot{x}_k p_k-\frac{1}{2m}p_k^2\right]}=\sqrt{\frac{2m\hbar\pi}{i\Delta t}}e^{\frac{i}{\hbar}\Delta t\frac{m}{2}\dot{x}_k^2}$. Therefore, we arrive at

$$\begin{aligned} i\hbar G &= \lim_{N\to\infty}\left(\frac{m}{2\pi i\hbar\Delta t}\right)^{\frac{N}{2}}\int\prod_{k=1}^{N-1}\mathrm{d}x_k\exp\left[\frac{i}{\hbar}\Delta t\sum_{\ell=0}^{N-1}\left(\frac{m}{2}\left(\frac{x_{\ell+1}-x_\ell}{\Delta t}\right)^2-V\left(x_\ell,t_\ell\right)\right)\right] \\ &= \int\mathcal{D}\left[x\left(t\right)\right]\exp\left[\frac{i}{\hbar}S\left(\left[x\left(t\right)\right],x_f,t_f,x_i,t_i\right)\right], \end{aligned} \tag{10}$$

where $\mathcal{D}\left[x\left(t\right)\right]=\lim_{N\to\infty}\left(\frac{m}{2\pi i\hbar\Delta t}\right)^{\frac{N}{2}}\prod_{k=1}^{N-1}\mathrm{d}x_k$, and

$$S\left(\left[x\left(t\right)\right],x_f,t_f,x_i,t_i\right)=\int_{t_i}^{t_f}\mathrm{d}t\left(\frac{m}{2}\dot{x}^2-V\left(x,t\right)\right) \tag{11}$$

is the action of the path $x\left(t\right)$ with the constraint that $x\left(t_f\right)=x_f$ and $x\left(t_i\right)=x_i$.

The formulation in (10) is known as the coordinate representation of the path integral. It answers our question of how each path interfere with each other. Each path contributes with a phase $e^{iS/\hbar}$, where the action S is measured in units of the Planck constant.

With the path integral formulation in (10), we can reinterpret Quantum Mechanics. Given the propagator (10), the time evolution of any state is determined through (4). Notice that this is equivalent to usual formulation in which one has to solve Schrödinger equation.

The path integral formulation is useful in many contexts, specially, for interacting systems where perturbation theory can be easily formulated. Philosophically, it helps us to "visualize" the quantum fluctuations. Usually, the classical path is the most contributing one for the propagator. In that case, we can interpret the real world as being classical with quantum fluctuations on top of it. Evidently, this picture has its limitation since there are phenomena in which the quantum character is dominant as in tunneling and in superconductivity.

A. Detour1: The free-particle propagator via path integral

In Sec. II A, we have computed the free-particle propagator by solving the Schrödinger equation for time evolution operator $\hat{U}$. It is instructive to perform the same task in the path integral formulation.

First, we will perform this calculation in a pragmatic way without paying much attention on the physical interpretation.

Consider the case $N=2$ in (10). We have to compute

$$\int\mathrm{d}x_1\exp\left[\frac{im}{2\hbar\Delta t}\left[\left(x_f-x_1\right)^2+\left(x_1-x_i\right)^2\right]\right]=\sqrt{\frac{2\pi i\hbar\Delta t}{m}\times\frac{1}{2}}\exp\left[\frac{im}{2\hbar\Delta t\times 2}\left(x_f-x_i\right)^2\right].$$

For the $N=3$, then we have that

$$\begin{aligned} \int\mathrm{d}x_1\mathrm{d}x_2\exp\left[\frac{im}{2\hbar\Delta t}\left[\left(x_f-x_2\right)^2+\left(x_2-x_1\right)^2+\left(x_1-x_i\right)^2\right]\right] &= \sqrt{\frac{2\pi i\hbar\Delta t}{m}\times\frac{1}{2}}\int\mathrm{d}x_1 e^{\frac{im}{2\hbar\Delta t}\left[\frac{1}{2}\left(x_f-x_1\right)^2+\left(x_1-x_i\right)^2\right]} \\ &= \sqrt{\left(\frac{2\pi i\hbar\Delta t}{m}\right)^2\times\frac{1}{2}\times\frac{2}{3}}e^{\frac{im}{2\hbar\Delta t}\times\frac{1}{3}\left(x_f-x_i\right)^2}. \end{aligned}$$

It seems there is a pattern arising. For the $N=k$ case, we use the induction hypothesis that

$$\int\prod_{\ell=1}^{k-1}\mathrm{d}x_\ell e^{\frac{im}{2\hbar\Delta t}\sum_{\ell=0}^{k-1}\left(x_{\ell+1}-x_\ell\right)^2}=\sqrt{\left(\frac{2\pi i\hbar\Delta t}{m}\right)^{\ell-1}\times\frac{1}{k}}e^{\frac{im}{2\hbar\Delta t}\times\frac{1}{k}\left(x_f-x_i\right)^2}.$$

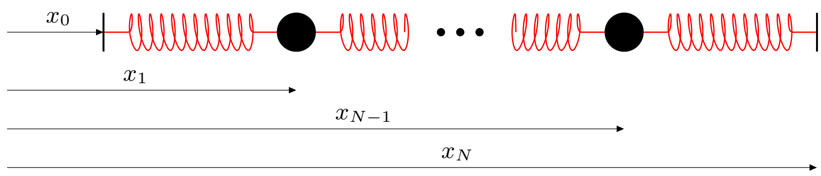

Figure 2: Chain of coupled harmonic oscillators.

For the next iteration $N = k+1$, we have to perform the integration

$$\int \mathrm{d}x_1 e^{\frac{im}{2\hbar\Delta t}\left[\frac{1}{k}(x_f-x_1)^2+(x_1-x_i)^2\right]} = \sqrt{\frac{2\pi i\hbar\Delta t}{m}\times\frac{k}{k+1}}e^{\frac{im}{2\hbar\Delta t}\times\frac{1}{k+1}(x_f-x_i)^2},$$

which confirms the induction hypothesis. Therefore,

$$\begin{aligned} i\hbar G &= \lim_{N\to\infty}\left(\frac{m}{2\pi i\hbar\Delta t}\right)^{\frac{N}{2}} \times \sqrt{\left(\frac{2\pi i\hbar\Delta t}{m}\right)^{\frac{N-1}{2}} \times \frac{1}{N} e^{\frac{im}{2\hbar\Delta t}\times\frac{1}{N}(x_f-x_i)^2}} \\ &= \lim_{N\to\infty}\left(\frac{m}{2\pi i\hbar\Delta t N}\right)^{\frac{1}{2}} e^{\frac{im}{\hbar 2}\times\frac{1}{\Delta t N}(x_f-x_i)^2} = \sqrt{\frac{m}{2\pi i\hbar\,(t_f-t_i)}}e^{\frac{i}{\hbar}\times\frac{m\left(x_f-x_i\right)^2}{2\left(t_f-t_i\right)}}, \end{aligned}$$

which recovers (5).

Notice that no information about the Schrödinger equation was used. However, the mathematical steps were much more "painful" in comparison to the usual formulation of quantum mechanics in Sec. II A.

B. Detour2: The free-particle propagator via path integral - reload

We now want redo the same calculation in a different manner. Notice we are dealing with the kinetic term $\propto \sum \dot{x}_k^2$. However, in the discrete limit, it can be viewed as a collection of $N-1$ coupled harmonic oscillators in 1D (see Fig. 2), the corresponding dimensionless potential energy being $U = \frac{1}{2}k\mathcal{V}$, where the "spring constant" $k = \frac{m}{\hbar\Delta t}$, and

$$\mathcal{V} = \sum_{\ell=0}^{N-1}\left(x_{\ell+1}-x_\ell\right)^2,$$

with x_0 and x_N fixed. The integration $\int\prod_{k=1}^{N-1}\mathrm{d}x_k$ means we are interested in all possible configurations of potential energy. Clearly, the lowest energy configuration (which is thus related to the classical path which minimizes the action) is that in which all particles are equally spaced, i.e., they are at their "equillibrium" position $x_\ell^{(\mathrm{eq})} = x_0 + \ell\left(\frac{x_N-x_0}{N}\right)$. Therefore, it is convenient to remove it out. For that, let us redefine the particle positions by $u_\ell = x_\ell - x_\ell^{(\mathrm{eq})}$. In this new variable, the potential energy becomes

$$\mathcal{V} = N\left(\frac{x_N-x_0}{N}\right)^2 + u_1^2 + \sum_{\ell=1}^{N-2}\left(u_{\ell+1}-u_\ell\right)^2 + u_{N-1}^2 = N\left(\frac{x_N-x_0}{N}\right)^2 + \mathbf{u}^T\mathbb{M}\mathbf{u},$$

where

$$\mathbb{M} = \begin{pmatrix} 2 & -1 & 0 & \cdots & 0 \\ -1 & 2 & -1 & \cdots & 0 \\ 0 & -1 & 2 & \cdots & \vdots \\ \vdots & \vdots & \vdots & \ddots & -1 \\ 0 & 0 & \cdots & -1 & 2 \end{pmatrix}$$

is a tridiagonal matrix, and $\mathbf{u}^T = \begin{pmatrix} u_1 & \ldots & u_{N-1} \end{pmatrix}$.

Notice the fluctuations around the "classical" configuration are weighted by the spring constant $k \propto m\hbar^{-1}$, i.e., we can somewhat quantify the weight of the quantum fluctuations by making an analogy with our springs. Stronger the spring constant, more suppressed are those configurations in which a particle deviates from its equilibrium (classical) position.

Notice moreover that $\mathbb{M}$ is easily diagonalized because the problem of Harmonic Oscillators with fixed ends is well known. The Eigenvectors are simply sines with wavelengths $\lambda_\alpha = \frac{2N}{\alpha}$, with $\alpha = 1, \ldots, N-1$, i.e., the wavevectors are $\mathbf{v}_\alpha$ with $v_{\ell,\alpha} \propto \sin\left(2\pi\ell/\lambda_\alpha\right)$. The normalization is $\sum_{\ell=1}^{N-1} \sin^2\left(\frac{\alpha\ell\pi}{N}\right) = \frac{1}{2}N$ (obtained from the sum of geometric series). Thus, $v_{\ell,\alpha} = \sqrt{\frac{2}{N}}\sin\left(\frac{\pi}{N}\alpha\ell\right)$. Applying these Eigenvectors on $\mathbb{M}$, we find the corresponding Eigenvalues $\omega_\alpha = 2 - 2\cos\left(\frac{\pi}{N}\alpha\right)$.

The potential can thus be rewritten as

$$\mathcal{V} = N\left(\frac{x_N - x_0}{N}\right)^2 + \mathbf{u}^T\left(\mathbb{V}\mathbb{D}\mathbb{V}^T\right)\mathbf{u} = N\left(\frac{x_N - x_0}{N}\right)^2 + \mathbf{z}^T\mathbb{D}\mathbf{z} = N\left(\frac{x_N - x_0}{N}\right)^2 + \sum_{\ell=1}^{N-1}\omega_\alpha z_\ell^2,$$

where the columns of $\mathbb{V}$ are the Eigenvectors $\mathbf{v}_\alpha$, $\mathbb{D}$ is a diagonal matrix in which $\mathbb{D}_{\alpha,\alpha} = \omega_\alpha$, and $\mathbf{z} = \mathbb{V}^T\mathbf{u}$. Since the transformation from $\mathbf{u} \to \mathbf{z}$ is a canonical one, then $\prod_{k=1}^{N-1} \mathrm{d}x_k = \prod_{k=1}^{N-1} \mathrm{d}u_k = \prod_{k=1}^{N-1} \mathrm{d}z_k$. The propagator can now be computed

$$\begin{aligned} i\hbar G &= \lim_{N\to\infty}\left(\frac{m}{2\pi i\hbar\Delta t}\right)^{\frac{N}{2}} e^{\frac{im\left(x_f - x_i\right)^2}{2\hbar\Delta t N}} \times \int\prod_{k=1}^{N-1}\mathrm{d}z_k e^{\frac{im}{2\hbar\Delta t}\sum_{\ell=1}^{N-1}\omega_\ell z_\ell^2} \\ &= \lim_{N\to\infty}\left(\frac{m}{2\pi i\hbar\Delta t}\right)^{\frac{N}{2}} e^{\frac{i}{\hbar}S_{\mathrm{cl}}} \times \left(\frac{2\pi i\hbar\Delta t}{m}\right)^{\frac{N-1}{2}} \times \frac{1}{\sqrt{\prod_\alpha\omega_\alpha}} = \lim_{N\to\infty}\left(\frac{m}{2\pi i\hbar\Delta t \mathrm{Det}\left(\mathbb{M}\right)}\right)^{\frac{1}{2}} e^{\frac{i}{\hbar}S_{\mathrm{cl}}}, \end{aligned}$$

where $\mathrm{Det}\left(\mathbb{M}\right) = \prod_\alpha \omega_\alpha$. (Indeed, the diagonalization of $\mathbb{M}$ is not crucial here, just its determinant.) The determinant can be obtained via induction. For a matrix of size $\ell = 1$, then $\mathrm{Det}\left(\mathbb{M}_1\right) = 2$. For size $\ell = 2$, then $\mathbb{M}_2 = \begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix}$, and the determinant is 3. For size $\ell = 3$, then $\mathrm{Det}\left(\mathbb{M}_3\right) = 4$. For a generic size ℓ, it is easy to show that $\mathrm{Det}\left(\mathbb{M}_\ell\right) = 2\mathrm{Det}\left(\mathbb{M}_{\ell-1}\right) - \mathrm{Det}\left(\mathbb{M}_{\ell-2}\right)$. Therefore, $\mathrm{Det}\left(\mathbb{M}_\ell\right) = \ell + 1$. As our matrix has size $\ell = N - 1$ and that $\Delta t N = \left(t_f - t_i\right)$, then we (again) recover the expected result (5).

IV. SEMICLASSICAL APPROACH

Having reformulated the quantum mechanics via the path integral approach, we might ask what kind of trajectories contribute the most for the propagator. For answering this question, let us consider for instance a system in which the action S is typically much larger than $\hbar$. By typically, we mean that for most of the paths $S \ggg \hbar$. Also, deviations from a typical path causes deviations in the action which are also much greater than $\hbar$, i.e., $\delta S \gg \hbar$. If that is the case, then most of these paths interfere with each other destructively because the phase varies so much that $e^{i\frac{S}{\hbar}}$ averages to zero. Therefore, there must be a set of paths that do not interfere destructively and dominate the sum $\int\mathcal{D}[x]$ over all paths. It is then clear that S must not vary much around these paths. Thus, there must be a special path around which δS vanishes (up to linear order in the deviation). In this case, it is said that the phase is stationary in this path. This must be the path that contributes the most for the propagator.

Let us suppose we find such special stationary-phase path and call it x_{cl}. Deviations from such path $\eta = x - x_{\mathrm{cl}}$ causes deviations on S that are specially small, i.e., $S - S_{\mathrm{cl}}$ must be a functional that is a quadratic function of $\delta[x]$, namely, $S - S_{\mathrm{cl}} = \frac{1}{2!}\int\mathrm{d}t\mathrm{d}t'\frac{\delta^2 S}{\delta x_{\mathrm{cl}}(t)\delta x_{\mathrm{cl}}(t')}\eta\left(t\right)\eta(t')$, where $\frac{\delta^2 S}{\delta x_{\mathrm{cl}}(t)\delta x_{\mathrm{cl}}(t')}$ represents the functional second derivative computed at the stationary phase path x_{cl}. If S were a function of a single variable x, then the second derivative would be simply $\left.\frac{\mathrm{d}^2 S}{\mathrm{d}x^2}\right|_{x=x_{\mathrm{cl}}}$. However, S is a functional, and thus, we have to deal with the calculus of variations.

In order to acquire more feeling, let us consider the case in which we simply divide the path in two steps (not necessarily of the same length) as in panel (a) of Fig. 1. In that case and considering a free particle, the propagator is given by (8)

$$\frac{1}{i\hbar}\int\mathrm{d}x_1 i\hbar G\left(x, t, x_1, t_1\right) \times i\hbar G\left(x_1, t_1, 0, 0\right) = \frac{1}{i\hbar}\sqrt{\frac{m}{2\pi i\hbar t_1}}\sqrt{\frac{m}{2\pi i\hbar\left(t - t_1\right)}}\int\mathrm{d}x_1 e^{i\frac{m}{2\hbar}\left(\frac{x_1^2}{t_1} + \frac{\left(x - x_1\right)^2}{t - t_1}\right)}.$$

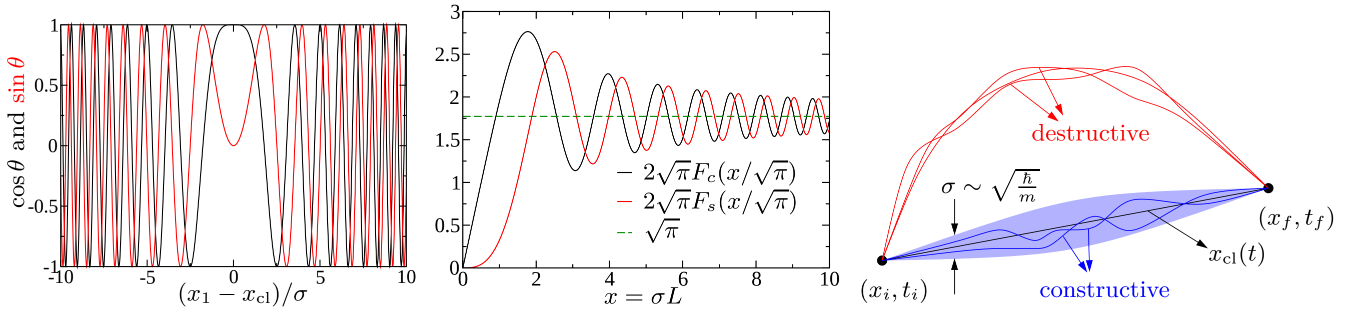

Figure 3: (Left) Phase contribution of each path x_1. (Middle) The integration over these phases which are Fresnel functions. (Right) Schematic of the paths contributing for the propagator. Inside the blue shaded region, the paths which contribute the most because the phase does not vary considerably. Outside this region, the phases vary considerably that they mostly interfere destructively by averaging away.

Let us have a better look at the integral

$$\int \mathrm{d}x_1 e^{i\frac{m}{2\hbar}\left(\frac{x_1^2}{t_1}+\frac{(x-x_1)^2}{t-t_1}\right)} = \int \mathrm{d}x_1 e^{i\frac{mt}{2\hbar t_1(t-t_1)}\left(x_1^2-2\frac{t_1}{t}xx_1+\frac{t_1}{t}x^2\right)} = \int \mathrm{d}x_1 e^{i\frac{mt}{2\hbar t_1(t-t_1)}\left(\left(x_1-\frac{t_1}{t}x\right)^2+\frac{t_1(t-t_1)}{t^2}x^2\right)}$$
$$= e^{i\frac{mx^2}{2t\hbar}}\int \mathrm{d}x_1 e^{i\frac{mt}{2\hbar t_1(t-t_1)}\left(x_1-\frac{t_1}{t}x\right)^2} = e^{i\frac{mx^2}{2t\hbar}}\int \mathrm{d}x_1 e^{i\frac{(x_1-x_{\rm cl})^2}{2\sigma^2}},$$

with $x_{\rm cl} = \frac{t_1}{t}x$ and $\sigma = \sqrt{\frac{\hbar t_1(t-t_1)}{mt}}$. The integration over x_1 can now be done without much effort, yielding $\sqrt{\frac{2\pi i\hbar(t-t_1)t_1}{mt}}e^{\frac{i}{\hbar}\times\frac{mx^2}{2t}}$, which is the well-known result (5). However, by simply performing the Gaussian integration we miss all the fun. Let us then have a closer look at the whole structure. Neglecting common factors, each path (represented by different values of x_1) contribute with the phase $e^{i\frac{(x_1-x_{\rm cl})^2}{2\sigma^2}} = e^{i\theta}$. Notice the phase θ increases for $|x_1 - x_{\rm cl}| \gg \sigma \sim \sqrt{\frac{\hbar}{m}}$. The real and imaginary part of the integrand are plotted in the left panel of Fig. 3.

In order to highlight the destructive interference of paths that are faraway from $x_{\rm cl}$, let us investigate the integral

$$\int_{-\infty}^{\infty}\mathrm{d}x_1 e^{i\frac{(x_1-x_{\rm cl})^2}{2\sigma^2}} = 2\lim_{L\to\infty}\int_0^L \mathrm{d}x e^{\frac{i}{2}\left(\frac{x}{\sigma}\right)^2} = 2\sigma\sqrt{\pi}\lim_{L\to\infty}\left(F_c\left(\sigma L\pi^{-1/2}\right)+iF_s\left(\sigma L\pi^{-1/2}\right)\right),$$

where $F_c(x) = \int_0^x \cos\left(\frac{\pi}{2}y^2\right)\mathrm{d}y$ and $F_s(x) = \int_0^x \sin\left(\frac{\pi}{2}y^2\right)\mathrm{d}y$ are the Fresnel functions which are plotted in the middle panel of Fig. 3. It is now clear that only the paths near the stationary one contributes. Notice the convergence of the Fresnel functions for large arguments. Indeed, for large arguments, we have that $F_c(x) \approx \frac{1}{2} + \frac{\pi}{x}\sin\left(\frac{\pi x^2}{2}\right)$ and $F_s(x) \approx \frac{1}{2} - \frac{\pi}{x}\cos\left(\frac{\pi x^2}{2}\right)$. The deviation from the convergent value falls as σ/L. [Notice it is not difficult to see why this error is of order L^{-1}. For instance, consider the integral $I = \int_L^\infty e^{-\alpha x^2}\mathrm{d}x$. By a simple variable changing, we have that

$$I = \frac{1}{\sqrt{\alpha}}\int_{\sqrt{\alpha}L}^{\infty} e^{-y^2}\mathrm{d}y = -\frac{1}{\sqrt{\alpha}}\int_{\sqrt{\alpha}L}^{\infty}\frac{1}{2y}\left(e^{-y^2}\right)'\mathrm{d}y = -\left.\frac{e^{-y^2}}{2\sqrt{\alpha}y}\right|_{\sqrt{\alpha}L}^{\infty} - \int_{\sqrt{\alpha}L}^{\infty}\frac{1}{2y^2}e^{-y^2}\mathrm{d}y$$
$$= \frac{1}{2\alpha L}e^{-\alpha L^2} - \mathcal{O}\left(\frac{1}{\alpha^2 L^3}e^{-\alpha L^2}\right).$$

Thus, for real positive α, the error is exponentially small. For pure imaginary α, the exponential is just a phase and the error is of order L^{-1}.]

A. Principle of least action for a single particle

Let us now be more serious find the special path $x_{\rm cl}(t)$. Our mathematical problem is to find the path $x_{\rm cl}$ that extremizes the action

$$S[x] = \int_{t_i}^{t_f}\mathrm{d}t\left(\frac{m}{2}\dot{x}^2 - V(x)\right),$$

with the constraints that $x(t_i) = x_i$ and $x(t_f) = x_f$. Let $x = x_{\rm cl} + \eta$, with the constraint that $\eta(t_i) = \eta(t_f) = 0$. Then, $\dot{x} = \dot{x}_{\rm cl} + \dot{\eta}$ and $\dot{x}^2 = \dot{x}_{\rm cl}^2 + 2\dot{x}_{\rm cl}\dot{\eta} + \mathcal{O}\left(\dot{\eta}^2\right)$. For small deviations, $V\left(x\right) = V(x_{\rm cl}) + \frac{\partial V}{\partial x}\big|_{x=x_{\rm cl}}\eta + \mathcal{O}\left(\eta^2\right)$. Plugging these results on S, we find that

$$\begin{aligned} S[x] &= \int {\rm d}t\left(\frac{m}{2}x_{\rm cl}^2 - V(x_{\rm cl})\right) + \int {\rm d}t\left(m\dot{x}_{\rm cl}\dot{\eta} - V'(x_{\rm cl})\eta\right) + \mathcal{O}\left(\dot{\eta}^2, \eta^2\right) \\ &= S_{\rm cl} + m\dot{x}_{\rm cl}\eta\big|_{t=t_i}^{t=t_f} - \int {\rm d}t\left(m\ddot{x}_{\rm cl} + V'(x_{\rm cl})\right)\eta\left(t\right) + \mathcal{O}\left(\dot{\eta}^2, \eta^2\right) = S_{\rm cl} + \delta S, \end{aligned}$$

where $\delta S = -\int {\rm d}t\left(m\ddot{x}_{\rm cl} + V'(x_{\rm cl})\right)\eta\left(t\right) + \mathcal{O}\left(\dot{\eta}^2, \eta^2\right)$. As we want $S_{\rm cl} = \int {\rm d}t\left(\frac{m}{2}x_{\rm cl}^2 - V(x_{\rm cl})\right)$ to be an extremum, then δS must vanish in the linear order of η. This happens whenever

$$m\ddot{x}_{\rm cl} = -\frac{\partial V}{\partial x_{\rm cl}},$$

which is Newton's 2nd law. Thus, $x_{\rm cl}$ is the classical path, as could have been anticipated from the physical intuition that classical mechanics must arise from quantum mechanics in the limit $\hbar \to 0$. Although classical mechanics is said to minimize the action (therefore the principle of the least action), we only proved that the action is an extremum, and that is the only necessary requirement.

B. Principle of least action for a generic system

We could have proceeded differently. Consider the general action

$$S = \int_{t_i}^{t_f} \mathcal{L}\left(t, x, \dot{x}\right){\rm d}t,$$

where x is a generalized coordinate. Again, our task is to find the optimal (stationary phase) path. Thus, let $x(t) = x_{\rm cl}(t) + \epsilon\eta\left(t\right)$. Then we apply the conventional wisdom of integral calculus to S with respect to ϵ. (Because now S is a function of the variable ϵ.) Setting $\frac{{\rm d}S}{{\rm d}\epsilon}\big|_{\epsilon=0} = 0$, we have that

$$\begin{aligned} 0 &= \int {\rm d}t\,\frac{{\rm d}\mathcal{L}}{{\rm d}\epsilon}\bigg|_{\epsilon=0} = \int {\rm d}t\left(\frac{\partial t}{\partial\epsilon}\frac{\partial\mathcal{L}}{\partial t} + \frac{\partial x}{\partial\epsilon}\frac{\partial\mathcal{L}}{\partial x} + \frac{\partial\dot{x}}{\partial\epsilon}\frac{\partial\mathcal{L}}{\partial\dot{x}}\right) \\ &= \int {\rm d}t\left(\eta\frac{\partial\mathcal{L}}{\partial x} + \dot{\eta}\frac{\partial\mathcal{L}}{\partial\dot{x}}\right) = \eta\frac{\partial\mathcal{L}}{\partial\dot{x}}\bigg|_{t=t_i}^{t=t_f} + \int {\rm d}t\eta\left(\frac{\partial\mathcal{L}}{\partial x} - \frac{\rm d}{{\rm d}t}\left(\frac{\partial\mathcal{L}}{\partial\dot{x}}\right)\right)\bigg|_{\epsilon=0}, \end{aligned}$$

from which we recover the Euler-Lagrange equation $\frac{\partial\mathcal{L}}{\partial x_{\rm cl}} - \frac{\rm d}{{\rm d}t}\left(\frac{\partial\mathcal{L}}{\partial\dot{x}_{\rm cl}}\right) = 0$. This can be easily generalized for any number of particles.

C. The classical path in the phase space representation

Had we chosen the phase space representation of the path integral (9), then the stationary phase path would arise in a different manner. Which manner is that? Let $S = \int {\rm d}t\left(\dot{x}p - H(x, p, t)\right)$ be the function we want to extremize. Setting $x = x_{\rm cl}(t) + \epsilon_1\eta_1(t)$ and $p = p_{\rm cl}(t) + \epsilon_2\eta_2(t)$, then we are looking for

$$\nabla_{\boldsymbol{\epsilon}}S|_{\boldsymbol{\epsilon}=0} = \left(\partial_{\epsilon_1}S, \partial_{\epsilon_2}S\right) = \mathbf{0} = \int {\rm d}t\left(-\eta_1\frac{\partial H}{\partial x} + \dot{\eta}_1 p, \eta_2\left(\dot{x} - \frac{\partial H}{\partial p}\right)\right).$$

Using the same trick of integration by parts for the $\dot{\eta}_1 p$ term, we arrive at the equations

$$\dot{p}_{\rm cl} = -\frac{\partial H}{\partial x_{\rm cl}} \text{ and } \dot{x}_{\rm cl} = \frac{\partial H}{\partial p_{\rm cl}},$$

which are at the Hamilton-Jacobi equations. Again, we arrive at the same conclusion that the classical path extremizes the action.

D. Stationary phase approximation

We are now in position to determine the semiclassical approach. This approach applies for the case in which $\hbar \to 0$ (more precisely, when the system is such that the actions of all paths are $S \gg \hbar$). Simply retaining the zeroth-order (which is the classical contribution for the propagator) term in the propagator is not enough because we want to keep some quantum fluctuations. We then keep the non-zero least (second) order in perturbation theory.

Mathematically, we are just interested in performing the integral $\int \mathcal{D}\left[x\right] e^{\frac{i}{\hbar}S[x]}$. For such, we choose the best integration variable which is $\eta\left(t\right) = x\left(t\right) - x_{\text{cl}}\left(t\right)$. Since this is a simple shift, then $\mathcal{D}\left[x\right] = \mathcal{D}\left[\eta\right]$. In addition, we Taylor expand the functional S up to second order in η,

$$S\left[x + x_{\text{cl}}\right] = S\left[x_{\text{cl}}\right] + \frac{1}{2}\int \mathrm{d}t\mathrm{d}t'\eta(t')\left(\frac{\delta^2 S}{\delta x(t)\delta x(t')}\right)\bigg|_{x=x_{\text{cl}}}\eta(t) + \mathcal{O}\left(\eta^3\right),$$

since the first order term $\int \mathrm{d}t\left(\frac{\delta S}{\delta x(t)}\right)\Big|_{x=x_{\text{cl}}}\eta(t) = 0$. We now have to define what exactly we mean by the second functional derivative $\frac{1}{2}\int \mathrm{d}t\mathrm{d}t'\eta(t')\left(\frac{\delta^2 S}{\delta x(t)\delta x(t')}\right)\Big|_{x=x_{\text{cl}}}\eta(t)$. We will follow the lines of thoughts of Secs. IV A and IV B.

Let us expand $S = \int \frac{m}{2}\dot{x}^2 - V\left(x\right)\mathrm{d}t$ up to second order in η. We have that $\dot{x}^2 = \dot{x}_{\text{cl}}^2 + 2\dot{x}_{\text{cl}}\dot{\eta} + \dot{\eta}^2$, and that $V\left(x\right) = V(x_{\text{cl}}) + V'(x_{\text{cl}})\eta + \frac{1}{2}V''(x_{\text{cl}})\eta^2$. Thus,

$$\begin{aligned} S\left[x\right] &= S[x_{\text{cl}}] + 0 + \int \mathrm{d}t\left(\frac{m}{2}\dot{\eta}^2 - \frac{1}{2}V''(x_{\text{cl}})\eta^2\right) \\ &= S[x_{\text{cl}}] + \frac{1}{2}\int \mathrm{d}t\eta(t)\left(-m\frac{\partial^2}{\partial t^2} - V''(x_{\text{cl}})\right)\eta\left(t\right), \end{aligned}$$

where we perform partial integration on the kinetic term: $\int \mathrm{d}t\dot{\eta}^2 = \eta\dot{\eta}\big|_{t=t_i}^{t=t_f} - \int \mathrm{d}t\eta\ddot{\eta}$. Therefore, we have found one meaning for the 2nd functional derivative symbol

$$\frac{1}{2}\int \mathrm{d}t\mathrm{d}t'\eta(t')\left(\frac{\delta^2 S}{\delta x(t)\delta x(t')}\right)\bigg|_{x=x_{\text{cl}}}\eta(t) = \frac{1}{2}\int \mathrm{d}t\eta(t)\left(-m\frac{\partial^2}{\partial t^2} - V''(x_{\text{cl}})\right)\eta\left(t\right). \tag{12}$$

Thus, in the semiclassical approach, we have that

$$i\hbar G = \int \mathcal{D}\left[x(t)\right] e^{\frac{i}{\hbar}S[x]} \approx e^{\frac{i}{\hbar}S[x_{\text{cl}}]}\int \mathcal{D}\left[\eta(t)\right] e^{\frac{i}{\hbar}\frac{1}{2}\int \mathrm{d}t\eta(t)\left(-m\frac{\partial^2}{\partial t^2} - V''(x_{\text{cl}})\right)\eta(t)}.$$

As we have seen for the $N = 2$ case in the free-particle action, the values of η that contribute are of order $\eta \sim \sqrt{\hbar}$. Mathematically, the semiclassical approach is thus a clever reduction of the path integral into a Gaussian integral.

Now, our task is to compute the Gaussian integral over $\mathcal{D}\left[\eta\right]$, it simply yields

$$i\hbar G_{\text{semiclassical}} = F(x_f, t_f, x_i, t_i)e^{\frac{i}{\hbar}S[x_{\text{cl}}]},$$

where the prefactor F is the result of the Gaussian integration [4]. Its interpretation is very important. Recalling that $\left|i\hbar G\right|^2$ is the probability density for finding the particle at (x_f, t_f) given that it was at (x_i, t_i), $\left|F\right|^2$ is exactly this quantity in the semiclassical approach. The result of in Gaussian integration is simply

$$\int \mathcal{D}\left[\eta(t)\right] e^{\frac{i}{\hbar}\frac{1}{2}\int \mathrm{d}t\eta(t)\left(-m\frac{\partial^2}{\partial t^2} - V''(x_{\text{cl}})\right)\eta(t)} = F = \left[\mathrm{Det}\left(\frac{-m\frac{\partial^2}{\partial t^2} - V''(x_{\text{cl}})}{2\pi i\hbar}\right)\right]^{-\frac{1}{2}}.$$

We now have to learn how to compute this determinant. But before doing so, let us see how it appears in a generic Lagragean. Writing $S = \int \mathrm{d}t\mathcal{L}\left(t, x, \dot{x}\right)$ and $x = x_{\text{cl}} + \epsilon\eta$, then

$$\begin{aligned} \frac{\mathrm{d}^2 S}{\mathrm{d}\epsilon^2} &= \int \mathrm{d}t\frac{\mathrm{d}}{\mathrm{d}\epsilon}\left(\frac{\partial t}{\partial \epsilon}\frac{\partial \mathcal{L}}{\partial t} + \frac{\partial x}{\partial \epsilon}\frac{\partial \mathcal{L}}{\partial x} + \frac{\partial \dot{x}}{\partial \epsilon}\frac{\partial \mathcal{L}}{\partial \dot{x}}\right) = \int \mathrm{d}t\frac{\mathrm{d}}{\mathrm{d}\epsilon}\left(\eta\frac{\partial \mathcal{L}}{\partial x} + \dot{\eta}\frac{\partial \mathcal{L}}{\partial \dot{x}}\right) \\ &= \int \mathrm{d}t\left(\frac{\partial x}{\partial \epsilon}\left(\eta\frac{\partial^2 \mathcal{L}}{\partial x^2} + \dot{\eta}\frac{\partial^2 \mathcal{L}}{\partial x\partial \dot{x}}\right) + \frac{\partial \dot{x}}{\partial \epsilon}\left(\eta\frac{\partial^2 \mathcal{L}}{\partial \dot{x}\partial x} + \dot{\eta}\frac{\partial^2 \mathcal{L}}{\partial \dot{x}^2}\right)\right) \\ &= \int \mathrm{d}t\left(\eta^2\frac{\partial^2 \mathcal{L}}{\partial x^2} + 2\eta\dot{\eta}\frac{\partial^2 \mathcal{L}}{\partial x\partial \dot{x}} + \dot{\eta}^2\frac{\partial^2 \mathcal{L}}{\partial \dot{x}^2}\right)\bigg|_{x=x_{\text{cl}}}. \end{aligned}$$

With that, we have found an alternative representation for Eq. (12) which is

$$\frac{1}{2}\int \mathrm{d}t\mathrm{d}t'\eta(t')\left(\frac{\delta^2 S}{\delta x(t)\delta x(t')}\right)\Bigg|_{x=x_{\mathrm{cl}}}\eta(t)=\frac{1}{2}\int \mathrm{d}t\left(\eta^2\frac{\partial^2\mathcal{L}}{\partial x^2}+2\eta\dot{\eta}\frac{\partial^2\mathcal{L}}{\partial x\partial\dot{x}}+\dot{\eta}^2\frac{\partial^2\mathcal{L}}{\partial\dot{x}^2}\right)\Bigg|_{x=x_{\mathrm{cl}}}. \tag{13}$$

Having found another representation for the second functional derivative of S, we can no longer delay the inevitable. How do we precisely compute the Gaussian integral? For that, let us step back and work on the discrete representation in Eq. (10). We then have to compute

$$\int\prod_{k=1}^{N-1}\mathrm{d}x_k\exp\left[\frac{i}{\hbar}\Delta t\sum_{\ell=0}^{N-1}\left(\frac{m}{2}\left(\frac{x_{\ell+1}-x_\ell}{\Delta t}\right)^2-V\left(x_\ell\right)\right)\right]\int\prod_{k=1}^{N-1}\mathrm{d}x_k\exp\left[\frac{i}{\hbar}S\left(x_0,\dots,x_N\right)\right],$$

where now S is a function of many variables. The first step, is to shift the many variables x_k from their classical (stationary phase) values $x_{\mathrm{cl},k}$. Thus, let us define $\eta_k=x_k-x_{\mathrm{cl},k}$. The second step is to expand S in powers of the deviations η_k. Up to second order, we have that

$$\begin{aligned}
S &\approx S_{\mathrm{cl}}+\sum_{\ell=1}^{N-1}\frac{\partial S}{\partial x_\ell}\Bigg|_{\mathbf{x}=\mathbf{x}_{\mathrm{cl}}}\eta_\ell+\frac{1}{2}\sum_{\ell,\ell'=1}^{N-1}\frac{\partial^2 S}{\partial x_\ell\partial x_{\ell'}}\Bigg|_{\mathbf{x}=\mathbf{x}_{\mathrm{cl}}}\eta_\ell\eta_{\ell'}\\
&=S_{\mathrm{cl}}+\Delta t\sum_{\ell=1}^{N-1}\left[-m\frac{\left(\frac{x_{\mathrm{cl},\ell+1}-x_{\mathrm{cl},\ell}}{\Delta t}\right)-\left(\frac{x_{\mathrm{cl},\ell}-x_{\mathrm{cl},\ell-1}}{\Delta t}\right)}{\Delta t}-V'\left(x_{\mathrm{cl}}\right)\right]\eta_\ell+\frac{1}{2}\boldsymbol{\eta}^T\mathbb{M}\boldsymbol{\eta}\\
&=S_{\mathrm{cl}}+\frac{1}{2}\boldsymbol{\eta}^T\mathbb{M}\boldsymbol{\eta},
\end{aligned}$$

where the linear order term vanishes identically, and

$$\mathbb{M}=\frac{m}{\Delta t}\begin{pmatrix}2&-1&0&\cdots&0\\-1&2&-1&\cdots&0\\0&-1&2&\cdots&\vdots\\\vdots&\vdots&\vdots&\ddots&-1\\0&0&\cdots&-1&2\end{pmatrix}-\Delta t\begin{pmatrix}V''\left(x_{\mathrm{cl},1}\right)&&&&\\&V''\left(x_{\mathrm{cl},2}\right)&&&\\&&V''\left(x_{\mathrm{cl},3}\right)&&\\&&&\ddots&\\&&&&V''\left(x_{\mathrm{cl},N-1}\right)\end{pmatrix}.$$

Finally, we can find the propagator

$$i\hbar G=e^{\frac{i}{\hbar}S_{\mathrm{cl}}}\times\lim_{N\to\infty}\left(\frac{m}{2\pi i\hbar\Delta t}\right)^{\frac{N}{2}}\int\prod_{k=1}^{N-1}\mathrm{d}\eta_k e^{\frac{i}{2\hbar}\boldsymbol{\eta}^T\mathbb{M}\boldsymbol{\eta}}=e^{\frac{i}{\hbar}S_{\mathrm{cl}}}\times\lim_{N\to\infty}\left(\frac{m}{2\pi i\hbar\Delta t}\right)^{\frac{N}{2}}\sqrt{\frac{(2\pi i\hbar)^{N-1}}{\mathrm{Det}\left(\mathbb{M}\right)}}.$$

We thus finally provided a way of computing

$$F=\left[\mathrm{Det}\left(\frac{-m\frac{\partial^2}{\partial t^2}-V''(x_{\mathrm{cl}})}{2\pi i\hbar}\right)\right]^{-\frac{1}{2}}=\lim_{N\to\infty}\left(\frac{m}{2\pi i\hbar\Delta t}\right)^{\frac{N}{2}}\sqrt{\frac{(2\pi i\hbar)^{N-1}}{\mathrm{Det}\left(\mathbb{M}\right)}}. \tag{14}$$

E. Application to the quadratic Lagrangeans

Notice the stationary phase (semiclassical) approach can be used to compute exactly any quadratic Lagrangean in x and $\dot{x}$. This is because $\frac{\delta^{(n)}S}{\delta x^n}=0$ for $n>2$.

The most general quadratic Lagrean has the form

$$\mathcal{L}=a(t)\dot{x}^2+b(t)\dot{x}x+c(t)x^2+d(t)\dot{x}+e(t)x,$$

where we neglect a possible constant term $f(t)$. In this case, we have that (this is not an approximation)

$$\begin{aligned}
S&=S_{\mathrm{cl}}+\int\mathrm{d}t\left(a(t)\dot{\eta}^2+b(t)\eta\dot{\eta}+c(t)\eta^2\right)\\
&=S_{\mathrm{cl}}+\Delta t\sum_{\ell=0}^{N-2}\left(a_\ell\left(\frac{\eta_{\ell+1}-\eta_\ell}{\Delta t}\right)^2+b_\ell\eta_\ell\left(\frac{\eta_{\ell+1}-\eta_\ell}{\Delta t}\right)+c_\ell\eta_\ell^2\right)\\
&=S_{\mathrm{cl}}+\frac{1}{2}\boldsymbol{\eta}^T\mathbb{M}\boldsymbol{\eta},
\end{aligned}$$

where the matrix $\mathbb{M}$ is such that their matrix elements are $M_{i,i} = 2c_i + \frac{2}{\Delta t}(2a_i - b_i)$, $M_{i,i+1} = M_{i+1,i} = \frac{1}{\Delta t}(-2a_i + b_i)$, and $M_{i,j} = 0$, otherwise. Here, the discretization of the function $a(t)$ are such that $a_\ell = a(t_i + \ell \frac{t_f - t_i}{N})$. [Analogously for the other function $b(t)$ and $c(t)$.] The factor F is computed as stated in (14).

An important class of Lagrangeans are of the type

$$\mathcal{L} = T - V = \frac{1}{2}m\dot{x}^2 + m\omega^2 x^{(\mathrm{eq})}x - \frac{1}{2}m\omega^2 x^2.$$

Therefore, we need only to compute

$$F = \lim_{N\to\infty}\left(\frac{m}{2\pi i\hbar\Delta t}\right)^{\frac{N}{2}}\left[\mathrm{Det}\left(2\pi i\hbar\mathbb{M}\right)\right]^{-\frac{1}{2}},$$

with

$$\mathbb{M} = \frac{m}{\Delta t}\begin{pmatrix} 2\cosh u & -1 & 0 & \cdots & 0 \\ -1 & 2\cosh u & -1 & \cdots & 0 \\ 0 & -1 & 2\cosh u & \cdots & \vdots \\ \vdots & \vdots & \vdots & \ddots & -1 \\ 0 & 0 & \cdots & -1 & 2\cosh u \end{pmatrix},$$

with $2\cosh u = 2 - (\omega\Delta t)^2$.

Let us now compute this determinant in a recursive way. For $N = 2$, then the matrix is a scalar and the determinant is simply $\mathrm{Det}\mathbb{M}_1 = 2\cosh u = e^u + e^{-u}$. For $N = 3$, we have $\mathbb{M}_2 = \begin{pmatrix} 2\cosh u & -1 \\ -1 & 2\cosh u \end{pmatrix}$, and the determinant is $4\cosh^2 u - 1 = e^{2u} + 1 + e^{-2u}$. For a generic matrix of size $\ell = N - 1$, it is easy to show that $\mathrm{Det}\mathbb{M}_\ell = 2\cosh u\,(\mathrm{Det}\mathbb{M}_{\ell-1}) - \mathrm{Det}\,(\mathbb{M}_{\ell-2})$. With this, we arrive at

$$\mathrm{Det}\mathbb{M}_\ell = \sum_{i=0}^{\ell} e^{(\ell-2i)u} = \frac{e^{(\ell+2)u} - e^{-\ell u}}{e^{2u} - 1} = \frac{\sinh\left((\ell+1)\,u\right)}{\sinh u}.$$

In our case, it is simple to compute u because $\Delta t \to 0$. Thus $2\cosh u = 2\cos(\omega\Delta t)$, i.e., $u = i\omega\Delta t$. Finally, we find that

$$\begin{aligned} F &= \lim_{N\to\infty}\left(\frac{m}{2\pi i\hbar\Delta t}\right)^{\frac{N}{2}}\sqrt{\frac{(2\pi i\hbar)^{N-1}}{\mathrm{Det}\,(\mathbb{M})}} = \lim_{N\to\infty}\left(\frac{m}{2\pi i\hbar\Delta t}\right)^{\frac{N}{2}}\sqrt{\frac{(2\pi i\hbar\Delta t)^{N-1}\sin\omega\Delta t}{m^{N-1}\sin(N\omega\Delta t)}} \\ &= \lim_{N\to\infty}\left(\frac{m}{2\pi i\hbar\Delta t}\right)^{\frac{1}{2}}\sqrt{\frac{\sin\omega\Delta t}{\sin(\omega t)}} = \sqrt{\frac{m\omega}{2\pi i\hbar\sin\omega t}}. \end{aligned} \tag{15}$$

For completeness, we compute the classical action

$$S_{\mathrm{cl}} = m\int_0^t \mathrm{d}t\left(\frac{1}{2}\dot{x}_{\mathrm{cl}}^2 + \omega^2 x^{(\mathrm{eq})}x_{\mathrm{cl}} - \frac{1}{2}\omega^2 x_{\mathrm{cl}}^2\right),$$

where $\ddot{x}_{\mathrm{cl}} = -\omega^2\left(x_{\mathrm{cl}} - x^{(\mathrm{eq})}\right)$, and thus $x_{\mathrm{cl}} = x^{(\mathrm{eq})} + A\cos\omega t + B\sin\omega t$, with $x(0) = x_i$ and $x(t) = x_f$. We then have that

$$\begin{aligned} S_{\mathrm{cl}} &= \frac{1}{2}m\omega^2\int_0^t \mathrm{d}t\left(x^{(\mathrm{eq})2} + \left(B^2 - A^2\right)\cos 2\omega t - 2AB\sin 2\omega t\right) \\ &= \frac{1}{2}m\omega^2\left(x^{(\mathrm{eq})2}t + \left(\frac{B^2 - A^2}{2\omega}\right)\sin 2\omega t + \frac{AB}{\omega}\left(\cos 2\omega t - 1\right)\right) \\ &= \frac{1}{2}m\omega\left[x^{(\mathrm{eq})2}\omega t + \left(x_f^2 + x_i^2 - 2x^{(\mathrm{eq})}\left(x_f + x_i - x^{(\mathrm{eq})}\right)\right)\cot\omega t - \frac{2\left(x_f - x^{(\mathrm{eq})}\right)\left(x_i - x^{(\mathrm{eq})}\right)}{\sin\omega t}\right]. \end{aligned} \tag{16}$$

F. Alternative approach to compute the prefactor F

In the semiclassical approximation we write the propagator as $i\hbar G_{\text{semiclassical}} = F e^{\frac{i}{\hbar}S[x_{\text{cl}}]}$, where the prefactor F is given by

$$F = \left[\text{Det}\left(\frac{-m\frac{\partial^2}{\partial t^2} - V''(x_{\text{cl}})}{2\pi i\hbar}\right)\right]^{-\frac{1}{2}},$$

and it contains all information about the quantum fluctuations about the classical action. We would like now to discuss an alternative approach to compute F in order to improve our understanding of the semiclassical approach. For simplicity, we write $V''(x_{\text{cl}}) = m\omega^2$ and discuss the solution of an (effective) harmonic oscillator. To evaluate the determinant, we look for the eigenvalues λ_n of the second-order differential operator $D(t) = -\left(\frac{\partial^2}{\partial t^2} + \omega^2\right)$, such that $\text{Det}(D(t)) = \prod_{n=1}^{\infty}\lambda_n$. To find these eigenvalues, we act with this operator on the fluctuations $\eta(t)$ and we are left with a differential equation subject to the (open) boundary conditions $\eta(0) = \eta(T) = 0$, where $T = t_f - t_i$. We thus look for solutions of the form

$$\eta(t) = \sum_{n=1}^{\infty} a_n \text{sen}\left(\frac{n\pi}{T}t\right),$$

such that

$$-\left(\frac{\partial^2}{\partial t^2} + \omega^2\right) a_n \text{sen}\left(\frac{n\pi}{T}t\right) = \underbrace{\left[\left(\frac{n\pi}{T}\right)^2 - \omega^2\right]}_{\lambda_n} a_n \text{sen}\left(\frac{n\pi}{T}t\right),$$

and

$$\lambda_n = \left(\frac{n\pi}{T}\right)^2 - \omega^2. \tag{17}$$

The determinant follows immediately

$$\begin{aligned}
\text{Det}\left(-\frac{\partial^2}{\partial t^2} - \omega^2\right) &= \prod_{n=1}^{\infty}\left[\left(\frac{n\pi}{T}\right)^2 - \omega^2\right] \\
&= \prod_{n=1}^{\infty}\left(\frac{n\pi}{T}\right)^2 \prod_{n=1}^{\infty}\left[1 - \left(\frac{\omega T}{n\pi}\right)^2\right] \\
&= C \times \frac{\sin(\omega T)}{\omega T}.
\end{aligned}$$

We introduced a constant factor C, independent of ω, and employed the identity $\prod_{n=1}^{\infty}\left[1 - (x/n\pi)^2\right] = \sin(x)/x$. The prefactor F is then given by

$$F = C'\sqrt{\frac{\omega T}{\sin(\omega T)}},$$

where the new factor C' absorbs the various constant terms. To fix the value of C' we recall that for $\omega = 0$ we must recover the free particle propagator, Eq. (5), and thus

$$F = \sqrt{\frac{m\omega}{2\pi i\hbar \sin(\omega T)}},$$

which naturally coincides with Eq. (15). For the Harmonic oscillator, the above expression is naturally exact because the potential truncates at second order.

Let us now briefly explore some interesting features of this solution. First, we notice that (again with $T = t_f - t_i$)

$$\begin{aligned}
&T < n\pi/\omega, \quad \lambda_n > 0 \ (\text{min}), \\
&T > n\pi/\omega, \quad \lambda_n < 0 \ (\text{max}),
\end{aligned}$$

and thus we see that the classical action is a minimum only at short times. This illustrates the fact we only require $S[x_{\rm cl}]$ to show vanishing first order variations. Another interesting feature is that F is singular at times $T = n\pi/\omega$. At these times, all trajectories pass through the points $\pm x_i$, $\eta = 0$ here, and these are known as focal points of the trajectories. The propagator is actually regular and we have

$$i\hbar G_{\rm semiclassical} = \begin{cases} \delta\left(x_f - x_i\right), & T = 2\pi m/\omega \\ \delta\left(x_f + x_i\right), & T = 2\pi\left(m+1\right)/\omega \end{cases},$$

where m is an integer, which is a directing consequence of the periodicity of the trajectories.

V. PATH INTEGRAL REPRESENTATION OF THE PARTITION FUNCTION

The partition function is a central quantity in statistical physics. Here, we show that it also has a path integral representation much alike the one for the time evolution of closed quantum systems. For simplicity, let us consider the canonical equilibrium partition function of a single particle system

$$Z = \sum_i e^{-\beta E_i} = \sum_\phi \left\langle \phi \left| e^{-\beta \hat{H}} \right| \phi \right\rangle = {\rm tr} e^{-\beta \hat{H}} = \int {\rm d}x \left\langle x \left| e^{-\beta \hat{H}} \right| x \right\rangle,$$

where $\beta^{-1} = k_B T$. Now, notice it can be rewritten as

$$Z = \int {\rm d}x_i \left. \left\langle x_i \left| e^{-\frac{i}{\hbar} t \hat{H}} \right| x_f \right\rangle \right|_{x_f = x_i, t = -i\hbar\beta} = \int {\rm d}x_i \hbar \mathcal{G}\left(x_i, x_i, \beta\right),$$

where

$$\mathcal{G}(x_f, x_i, \beta) = \hbar^{-1} \left\langle x_f \left| e^{-\beta \hat{H}} \right| x_i \right\rangle = iG\left(x_f, t, x_i, 0\right),$$

is called the propagator in the imaginary time $t = -i\hbar\beta$.

It is now clear that there is a relation between the real time evolution of a quantum system and its equilibrium partition function.

We now investigate the corresponding imaginary time propagator. Starting from (9), we have that

$$\begin{aligned} \hbar\mathcal{G}(x_f, x_i, \beta) &= \lim_{N\to\infty} \int \prod_{k=1}^{N-1} {\rm d}x_k \prod_{l=0}^{N-1} \frac{{\rm d}p_l}{2\pi\hbar} \exp\left[\frac{i}{\hbar}\Delta t \sum_{\ell=0}^{N-1} \left(\left(\frac{x_{\ell+1} - x_\ell}{\Delta t}\right) p_\ell - H\left(p_\ell, x_\ell\right)\right)\right] \\ &= \int \mathcal{D}\left[q\left(t\right)\right] \exp\left[\frac{i}{\hbar}\int_0^t {\rm d}t' \left(\frac{\partial x}{\partial t'} p - H\left(p, x\right)\right)\right] = \int \mathcal{D}\left[q\left(t\right)\right] e^{-\frac{1}{\hbar} S_E([x],[p])}, \end{aligned}$$

where $x_0 = x_i$, $x_N = x_f$, and $\Delta t = \frac{t}{N} = -i\frac{\hbar\beta}{N}$. Defining $\tau = it'$, we find that

$$S_E\left([x],[p]\right) = -i\int_0^{-i\hbar\beta} {\rm d}t' \left(\frac{\partial x}{\partial t'} p - H\left(p, x\right)\right) = \int_0^{\hbar\beta} {\rm d}\tau \left(-i\frac{\partial x}{\partial \tau} p + H\left(p, x\right)\right) = \int_0^{\hbar\beta} {\rm d}\tau \left(-i\dot{x}p + H\left(p, x\right)\right).$$

The action S_E is called the Euclidean action in the phase space. Notice τ represents a real Euclidean "time." We can integrate over the momenta p_ℓ and obtain the Euclidean action in the coordinate space. Alternatively, we can use Eq. (10) and arrive at

$$\begin{aligned} \hbar\mathcal{G}(x_f, x_i, \beta) &= \lim_{N\to\infty} \left(\frac{m}{2\pi i\hbar\Delta t}\right)^{\frac{N}{2}} \int \prod_{k=1}^{N-1} {\rm d}x_k \exp\left[\frac{i}{\hbar}\Delta t \sum_{\ell=0}^{N-1} \left(\frac{m}{2}\left(\frac{x_{\ell+1} - x_\ell}{\Delta t}\right)^2 - V\left(x_\ell\right)\right)\right] \\ &= \lim_{N\to\infty} \left(\frac{m}{2\pi\hbar\Delta\tau}\right)^{\frac{N}{2}} \int \prod_{k=1}^{N-1} {\rm d}x_k \exp\left[-\frac{1}{\hbar}\Delta\tau \sum_{\ell=0}^{N-1} \left(\frac{m}{2}\left(\frac{x_{\ell+1} - x_\ell}{\Delta\tau}\right)^2 + V\left(x_\ell\right)\right)\right] \\ &= \int \mathcal{D}\left[x\right] e^{-\frac{1}{\hbar}\int {\rm d}\tau\left(\frac{m}{2}\dot{x}^2 + V(x)\right)} = \int \mathcal{D}\left[x\right] e^{-\frac{1}{\hbar} S_E([x])}, \end{aligned} \tag{18}$$

where the Euclidean action is $S_E = \int {\rm d}\tau\left(T + V\right)$. Notice the difference with respect to the conventional (Minkowski) action in Eq. (11) $S_M \equiv S = \int {\rm d}t\mathcal{L} = \int {\rm d}t\left(T - V\right)$. So, the Euclidean action is obtained from the usual Minkowski action simply by changing the sign of the potential. Thus, the Euclidean action is directly related to the Hamiltonian of the related classical theory.

It is interesting to note that in the great majority of the cases, we are interested in some mean value. In statistical mechanics, this means we will be interested in some derivative of $\ln Z$. In that case, the normalization term $\left(\frac{m}{2\pi\hbar\Delta\tau}\right)^{\frac{N}{2}}$ becomes irrelevant.

Finally, we rewrite the equilibrium partition function as

$$Z = \sum_{\text{all periodic paths}} e^{-\frac{1}{\hbar}S_E} = \int \mathcal{D}\left[x\left(\tau\right)\right] e^{-\frac{1}{\hbar}\int_0^{\hbar\beta}(T+V)\mathrm{d}\tau} = \int \mathcal{D}\left[x\left(\beta'\right)\right] e^{-\int_0^{\beta}(T+V)\mathrm{d}\tau'}, \tag{19}$$

where the paths are such that $x_i = x_f$ [or $x\left(0\right) = x\left(\hbar\beta\right)$]. In the last passage, we have changed the integration variable $\tau \to \tau'\hbar$. In this way, the Euclidean action becomes dimensionless and $\hbar$ drops out from the calculation. The difference is that the "time" τ' has units of inverse of energy.

Notice that the path integral formalism unveils a deep connection between classical statistical mechanics and quantum mechanics (as well as between classical and quantum statistical mechanics). Without the path integral formalism, a watchful one could have noticed that computing the equilibrium partition function $Z = \mathrm{tr}e^{-\beta\hat{H}}$ of a quantum system is equivalent (via an analytical continuation $\beta \to it/\hbar$) to compute the real time evolution of this system along all possible closed loops. However, the path integral formulation tells us that this quantum partition function is equal to the partition function of some different (but related) classical system. This fact builds a bridge between the areas of field theory and statistical physics which have benefited from each other over the years.

Before we start computing the partition function in the path-integral formalism, let us finally compare Z in (19) with the partition function of a linear string of length L in some external potential $V(x)$. For small displacements $u(x)$ (with $0 < x < L$), the system energy for some configuration $u(x)$ is $\int_0^L \mathrm{d}x \left(\sigma\dot{u}^2 + v(u)\right) + \text{const}$. The first term accounts for the elastic energy and σ is the string tension. Thus, summing over all possible configurations $\mathcal{D}\left[u(x)\right]$, we have that

$$Z_{\text{cl}} = \int \mathcal{D}\left[u(x)\right] e^{-\beta_{\text{cl}}\int_0^L \mathrm{d}x(t+v)} = \int \mathcal{D}\left[u(x)\right] e^{-\frac{\beta_{\text{cl}}}{\xi}\int_0^L \mathrm{d}x(T+V)} = \int \mathcal{D}\left[u(t)\right] e^{-\beta_{\text{cl}}\frac{c}{\xi}\int_0^{L/c}\mathrm{d}t(T+V)},$$

where we have inserted two new quantities: some velocity c (from which $x = ct$) and some correlation length ξ (from which we defined the density of potential energy $v(u) = V(u)/\xi$, and the density of elastic energy $t = T/\xi$).

Comparing with (19), we have that the effective classical temperature is $k_B T_{\text{cl}}\frac{c}{\xi} = \beta_{\text{cl}}^{-1} = \hbar$ and the system length in the new imaginary-time dimension is $L = c\hbar\beta$.

Notice that (19) was derived for a system constituted by a single quantum particle. The path-integral formulation tells us that this is equivalent to a classical system of interacting many particles. The size of this system is L which is formally infinite in the zero-temperature limit $\beta \to \infty$. The effective classical temperature is solely due to quantum fluctuations since $T_{\text{cl}} \propto \hbar$. Evidently, the precise analogy is model dependent since the length ξ and speed c constants may not be universal and depends on how one takes the continuum limit from the quantum to the classical formulation. For now, we arrive at the interesting conclusion that a zero-temperature quantum system correspond to a classical one in $d+1$ dimensions. We will discuss this quantum-to-classical mapping latter on.

A. The quantum Harmonic Oscillator

Let us illustrate the connection between the real time evolution of a quantum system and its partition function taking the 1D quantum Harmonic Oscillator, the Hamiltonian of which is $\hat{H} = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)$, as an example.

Using the conventional methods of statistical physics, we simply have that

$$Z = \mathrm{tr}e^{-\beta\hat{H}} = \sum_{n=0}^{\infty} e^{-\beta\hbar\omega\left(n+\frac{1}{2}\right)} = e^{-\frac{\beta\hbar\omega}{2}}\left(\frac{1}{1-e^{-\beta\hbar\omega}}\right) = \frac{1}{2\sinh\frac{1}{2}\beta\hbar\omega}.$$

However, this result can be obtained via the more "painful" path-integral way. Gladly, we can already start with the real time results (15) and (16). Using that $x_i = x_f = x_0$, $x^{(\text{eq})} = 0$, and that $t = -i\hbar\beta$, we have that

$$\hbar\mathcal{G}(x_0, x_0, \beta) = \sqrt{\frac{m\omega}{2\pi i\hbar\sin\omega t}} e^{\frac{i}{\hbar}\frac{1}{2}m\omega\left[2x_0^2\cot\omega t - \frac{2x_0x_0}{\sin\omega t}\right]} = \sqrt{\frac{m\omega}{2\pi\hbar\sinh\beta\hbar\omega}} e^{-\frac{1}{\hbar}m\omega x_0^2\left(\frac{\cosh\beta\hbar\omega - 1}{\sinh\beta\hbar\omega}\right)}. \tag{20}$$

The partition function is now obtained by a simple Gaussian integration over x_0:

$$Z=\int \mathrm{d}x_0\hbar\mathcal{G}\left(x_0,x_0,\beta\right)=\sqrt{\frac{m\omega}{2\pi\hbar\sinh\beta\hbar\omega}}\times\sqrt{\frac{\pi\hbar\sinh\beta\hbar\omega}{m\omega\left(\cosh\beta\hbar\omega-1\right)}}=\frac{1}{2\sinh\frac{1}{2}\beta\hbar\omega}.$$

We can now perform an analytical continuation from the Euclidean time to the Minkowski time $\beta\to it/\hbar$. Then

$$Z=\frac{1}{2\sinh\frac{1}{2}\beta\hbar\omega}=\sum_{n=0}^{\infty}e^{-\beta\hbar\omega\left(n+\frac{1}{2}\right)}=\sum_{n=0}^{\infty}e^{-i\omega t\left(n+\frac{1}{2}\right)}=\sum_{n=0}^{\infty}e^{\frac{1}{i\hbar}tE_n}=\mathrm{tr}e^{\frac{1}{i\hbar}t\hat{H}},$$

where $E_n=\hbar\omega\left(n+\frac{1}{2}\right)$ is the spectrum of the Harmonic Oscillator.

VI. QUANTUM-CLASSICAL MAPPING

We now want to further explore the relation between quantum statistical mechanics (or, equivalently, quantum mechanics in the imaginary time) and classical statistical mechanics. Although this subject could fit as a subsection of the previous section, we thought that this relation is so important that it deserves its own section.

At zero-temperature, the fluctuations on a quantum system are only due to its zero-point fluctuations, i.e., the fluctuation are exclusively of quantum character due to the uncertainty principle. What is the corresponding classical system? First, notice the length of the imaginary-time dimension is $\propto\beta\to\infty$. Therefore, the corresponding classical system leaves in $d+1$ dimensions. Also, the classical system is an interacting one but we leave this part for later. In addition, a classical system does not have quantum fluctuations. What is its source of fluctuations, then? It can only be of thermal nature. Thus, the strength of the zero-point fluctuations must correspond to an effective temperature in the classical counterpart.

What are the changes when we now consider the case of finite-temperature. In that case, the new imaginary time dimension is no longer infinite. As it is well known from classical statical mechanics, thermal fluctuations are stronger in lesser dimensions. Therefore, thermal fluctuations in the quantum systems correspond to a smaller classical system in the imaginary-time dimension.

In order to make the above statements more precise and less abstract, let us illustrate them by considering the simple model of a localized spin-1/2 particle in a longitudinal B and transversal h field

$$\hat{H}=-h\hat{\sigma}^x-B\hat{\sigma}^z, \tag{21}$$

where the $\hat{\sigma}^x=\begin{pmatrix}0&1\\1&0\end{pmatrix}$ and $\hat{\sigma}^z=\begin{pmatrix}1&0\\0&-1\end{pmatrix}$ are Pauli matrices representing the spin-1/2 particle (or a generic two-level system). We can view this problem in the following way. The longitudinal field splits the degeneracy between the $|\uparrow\rangle$ and $|\downarrow\rangle$ states. The transverse field induces flips between these states and hence can be regard as the strength of the quantum fluctuation.

A. Analyzing the problem in the quantum realm

Let us diagonalize this Hamiltonian in the Schrödinger formalism. Notice $\hat{H}=-\mathbf{h}_{\rm tot}\cdot\hat{\boldsymbol{\sigma}}=-h_{\rm tot}\hat{\sigma}^n$, where $\mathbf{h}_{\rm tot}=(h,0,B)=h_{\rm tot}\hat{n}=h_{\rm tot}\left(\sin\theta\hat{x}+\cos\theta\hat{z}\right)$, with $h_{\rm tot}=\sqrt{h^2+B^2}$ and $\tan\theta=\frac{h}{B}$. Therefore, the spectrum is $E_{\nearrow}=-h_{\rm tot}$ and $E_{\swarrow}=h_{\rm tot}$. The Eigenstates are the basis of $\hat{\sigma}^n=\sin\theta\hat{\sigma}^x+\cos\theta\hat{\sigma}^z$:

$$\begin{pmatrix}|\nearrow\rangle\\|\swarrow\rangle\end{pmatrix}=\begin{pmatrix}\sin\frac{1}{2}\theta&-\cos\frac{1}{2}\theta\\\cos\frac{1}{2}\theta&\sin\frac{1}{2}\theta\end{pmatrix}\begin{pmatrix}|\uparrow\rangle\\|\downarrow\rangle\end{pmatrix},\Rightarrow\begin{pmatrix}|\uparrow\rangle\\|\downarrow\rangle\end{pmatrix}=\begin{pmatrix}\sin\frac{1}{2}\theta&\cos\frac{1}{2}\theta\\-\cos\frac{1}{2}\theta&\sin\frac{1}{2}\theta\end{pmatrix}\begin{pmatrix}|\nearrow\rangle\\|\swarrow\rangle\end{pmatrix}.$$

The partition function is simply

$$Z=2\cosh\beta h_{\rm tot}. \tag{22}$$

The imaginary time propagators are

$$\begin{aligned}\hbar\mathcal{G}(\uparrow,\uparrow,\beta)&=\left\langle\uparrow\left|e^{-\beta\hat{H}}\right|\uparrow\right\rangle=e^{\beta h_{\rm tot}}\left|\langle\uparrow\mid\nearrow\rangle\right|^2+e^{-\beta h_{\rm tot}}\left|\langle\uparrow\mid\swarrow\rangle\right|^2\\&=e^{\beta h_{\rm tot}}\sin^2\frac{1}{2}\theta+e^{-\beta h_{\rm tot}}\cos^2\frac{1}{2}\theta,\\\hbar\mathcal{G}(\downarrow,\downarrow,\beta)&=e^{\beta h_{\rm tot}}\cos^2\frac{1}{2}\theta+e^{-\beta h_{\rm tot}}\sin^2\frac{1}{2}\theta.\end{aligned}$$

Again, we can compute $Z = \hbar\mathcal{G}(\uparrow,\uparrow,\beta) + \hbar\mathcal{G}(\downarrow,\downarrow,\beta) = 2\cosh\beta h_{\text{tot}}$.

The free energy is

$$f = -\frac{1}{\beta}\ln Z = -\frac{1}{\beta}\left[\ln\left(\cosh\beta h_{\text{tot}}\right) + \ln 2\right].$$

Therefore, the (longitudinal) magnetization is

$$m = -\frac{\partial}{\partial B}f = \frac{1}{\beta}\tanh\beta h_{\text{tot}} \times \frac{\beta B}{\sqrt{h^2+B^2}} = \frac{B}{h_{\text{tot}}}\tanh\beta h_{\text{tot}}. \tag{23}$$

Thus, at the zero temperature limit ($\beta \to \infty$),

$$m_{T=0} \to \frac{B}{h_{\text{tot}}}. \tag{24}$$

(Notice that the h is responsible for diminishing m, i.e., it parameterizes the strength of the quantum fluctuations.)

The magnetic susceptibility is also computed:

$$\chi = \frac{\partial}{\partial B}m\bigg|_{B\to 0} = \frac{1}{h}\tanh\beta h. \tag{25}$$

Then, at zero temperature,

$$\chi_{T=0} = \frac{1}{h}. \tag{26}$$

We now compute the connected correlation function $G(t) = \langle\hat{\sigma}^z(0)\,\hat{\sigma}^z(t)\rangle - \langle\hat{\sigma}^z(0)\rangle\langle\hat{\sigma}^z(t)\rangle$. The temporal mean value of σ is the magnetization itself

$$\langle\hat{\sigma}^z(t)\rangle = \frac{1}{Z}\text{tr}\left\{e^{\frac{i}{\hbar}\hat{H}t}\hat{\sigma}^z e^{-\frac{i}{\hbar}\hat{H}t}e^{-\beta\hat{H}}\right\} = \frac{1}{Z}\text{tr}\left\{\hat{\sigma}^z e^{-\frac{i}{\hbar}Ht}e^{-\beta H}e^{\frac{i}{\hbar}Ht}\right\} = \frac{1}{Z}\text{tr}\left\{\hat{\sigma}^z e^{-\beta H}\right\} = m.$$

The two-body correlation, however, is time-dependent:

$$\langle\hat{\sigma}^z(0)\,\hat{\sigma}^z(t)\rangle = \frac{1}{Z}\text{tr}\left\{\hat{\sigma}^z e^{\frac{i}{\hbar}\hat{H}t}\hat{\sigma}^z e^{-\frac{i}{\hbar}\hat{H}t}e^{-\beta\hat{H}}\right\}.$$

The above trace we will be computed in the basis of $\hat{\sigma}^{\hat{n}}$. Thus,

$$\begin{aligned}
\left\langle\nearrow\left|\hat{\sigma}^z e^{\frac{i}{\hbar}\hat{H}t}\hat{\sigma}^z e^{-\frac{i}{\hbar}\hat{H}t}e^{-\beta\hat{H}}\right|\nearrow\right\rangle &= e^{\left(\frac{i}{\hbar}t+\beta\right)h_{\text{tot}}}\left\langle\nearrow\left|\hat{\sigma}^z e^{\frac{i}{\hbar}\hat{H}t}\hat{\sigma}^z\right|\nearrow\right\rangle,\\
&= -\cos\theta e^{\left(\frac{i}{\hbar}t+\beta\right)h_{\text{tot}}}\left\langle\nearrow\left|\hat{\sigma}^z e^{\frac{i}{\hbar}\hat{H}t}\right|\nearrow\right\rangle + \sin\theta e^{\left(\frac{i}{\hbar}t+\beta\right)h_{\text{tot}}}\left\langle\nearrow\left|\hat{\sigma}^z e^{\frac{i}{\hbar}\hat{H}t}\right|\swarrow\right\rangle,\\
&= -\cos\theta e^{\beta h_{\text{tot}}}\left\langle\nearrow\left|\hat{\sigma}^z\right|\nearrow\right\rangle + \sin\theta e^{\left(2\frac{i}{\hbar}t+\beta\right)h_{\text{tot}}}\left\langle\nearrow\left|\hat{\sigma}^z\right|\swarrow\right\rangle,\\
&= \cos^2\theta e^{\beta h_{\text{tot}}} + \sin^2\theta e^{\left(2\frac{i}{\hbar}t+\beta\right)h_{\text{tot}}}.
\end{aligned}$$

and

$$\begin{aligned}
\left\langle\swarrow\left|\hat{\sigma}^z e^{\frac{i}{\hbar}\hat{H}t}\hat{\sigma}^z e^{-\frac{i}{\hbar}\hat{H}t}e^{-\beta\hat{H}}\right|\swarrow\right\rangle &= e^{-\left(\frac{i}{\hbar}t+\beta\right)h_{\text{tot}}}\left\langle\swarrow\left|\hat{\sigma}^z e^{\frac{i}{\hbar}\hat{H}t}\hat{\sigma}^z\right|\swarrow\right\rangle,\\
&= \cos\theta e^{-\left(\frac{i}{\hbar}t+\beta\right)h_{\text{tot}}}\left\langle\swarrow\left|\hat{\sigma}^z e^{\frac{i}{\hbar}\hat{H}t}\right|\swarrow\right\rangle + \sin\theta e^{-\left(\frac{i}{\hbar}t+\beta\right)h_{\text{tot}}}\left\langle\swarrow\left|\hat{\sigma}^z e^{\frac{i}{\hbar}\hat{H}t}\right|\nearrow\right\rangle,\\
&= \cos^2\theta e^{-\beta h_{\text{tot}}} + \sin^2\theta e^{-\left(2\frac{i}{\hbar}t+\beta\right)h_{\text{tot}}}.
\end{aligned}$$

Therefore,

$$\begin{aligned}
\langle\hat{\sigma}^z(0)\,\hat{\sigma}^z(t)\rangle &= \frac{2}{Z}\left[\cos^2\theta\cosh\beta h_{\text{tot}} + \sin^2\theta\cosh\left(-2\tau\hbar^{-1}+\beta\right)h_{tot}\right],\\
&= \cos^2\theta + \sin^2\theta\frac{\cosh\left(-2\tau\hbar^{-1}+\beta\right)h_{\text{tot}}}{\cosh\beta h_{\text{tot}}} = \left(\frac{B}{h_{\text{tot}}}\right)^2 + \left(\frac{h}{h_{\text{tot}}}\right)^2\frac{\cosh\left(-2\tau\hbar^{-1}+\beta\right)h_{\text{tot}}}{\cosh\beta h_{\text{tot}}},
\end{aligned}$$

with $\tau = -it$. Therefore,

$$G(t) = \left(\frac{B}{h_{\mathrm{tot}}}\right)^2 \frac{1}{\cosh^2 \beta h_{\mathrm{tot}}} + \left(\frac{h}{h_{\mathrm{tot}}}\right)^2 \frac{\cosh\left(-2\tau\hbar^{-1} + \beta\right) h_{\mathrm{tot}}}{\cosh \beta h_{\mathrm{tot}}}. \tag{27}$$

In the limit of $T \to 0$,

$$\begin{aligned} G(\tau) &\to \left(\frac{h}{h_{\mathrm{tot}}}\right)^2 \frac{e^{\left(-2\tau\hbar^{-1}+\beta\right)h_{\mathrm{tot}}}}{e^{\beta h_{\mathrm{tot}}}} \\ &= \left(\frac{h}{h_{\mathrm{tot}}}\right)^2 e^{-\tau/\xi_\tau}, \text{ with } \xi_\tau = \frac{\hbar}{2h_{\mathrm{tot}}} = \frac{\hbar}{2\sqrt{h^2+B^2}}. \end{aligned} \tag{28}$$

For $B = 0$,

$$\xi_\tau = \frac{\hbar}{2h}, \text{ and } G(\tau, B=0) = e^{-\tau/\xi_\tau} = e^{-2\frac{\tau h}{\hbar}}. \tag{29}$$

We now compute the same quantities in the classical path-integral formulation.

B. Analyzing the problem in the classical realm

Our first task is to derive the path integral for the Hamiltonian partition function. Choosing the partition function to be represented in the $\hat{\sigma}^z$ basis, i.e., $\hat{\sigma}^z\left|\uparrow\right\rangle = \left|\uparrow\right\rangle$ and $\hat{\sigma}^z\left|\downarrow\right\rangle = -\left|\downarrow\right\rangle$, we then have that

$$\begin{aligned} Z &= \mathrm{tr} e^{-\beta\hat{H}} = \sum_{\sigma=\uparrow,\downarrow} \left\langle \sigma \left| e^{-\beta\hat{H}} \right| \sigma \right\rangle, \\ &= \sum_{\sigma_1,\ldots,\sigma_N} \left\langle \sigma_0 \left| e^{-\frac{\beta}{N}\hat{H}} \right| \sigma_1 \right\rangle \left\langle \sigma_1 \left| e^{-\frac{\beta}{N}H} \right| \sigma_2 \right\rangle \ldots \left\langle \sigma_{N-1} \left| e^{-\frac{\beta}{N}H} \right| \sigma_N \right\rangle, \end{aligned}$$

where $\sigma_0 = \sigma_N$, and we will take the $N \to \infty$ limit. In this limit, we have that $e^{-\frac{\beta}{N}\hat{H}} = e^{\frac{\beta}{N}h\hat{\sigma}^x} e^{B\frac{\beta}{N}\hat{\sigma}^z}$. We now have to deal with

$$\left\langle \sigma_{k-1} \left| e^{\frac{\beta}{N}h\hat{\sigma}^x} e^{B\frac{\beta}{N}\hat{\sigma}^z} \right| \sigma_k \right\rangle = \left[\sum_{\sigma^x=\rightarrow,\leftarrow} e^{\frac{\beta}{N}h\sigma^x} \left\langle \sigma_{k-1} | \sigma^x \right\rangle \left\langle \sigma^x | \sigma_k \right\rangle\right] e^{\frac{\beta}{N}B\sigma_k},$$

where we have inserted $\mathbb{I} = \sum_{\sigma^x} \left|\sigma^x\right\rangle\left\langle\sigma^x\right|$. We now want to conveniently evaluate $\sum_{\sigma^x} e^{\frac{\beta}{N}h\sigma^x} \left\langle \sigma_{k-1} | \sigma^x \right\rangle \left\langle \sigma^x | \sigma_k \right\rangle$. Since $\left\langle \uparrow | \rightarrow \right\rangle = \left\langle \downarrow | \rightarrow \right\rangle = \left\langle \uparrow | \leftarrow \right\rangle = -\left\langle \downarrow | \leftarrow \right\rangle = 1/\sqrt{2}$, it is easy to see that

$$\sum_{\sigma^x} e^{\frac{\beta}{N}h\sigma^x} \left\langle \sigma_{k-1} | \sigma^x \right\rangle \left\langle \sigma^x | \sigma_k \right\rangle = \frac{1}{2}\left(e^{\frac{\beta}{N}h} + \sigma_{k-1}\sigma_k e^{-\frac{\beta}{N}h}\right).$$

However, for convenience, we wish to express it as $\exp\left\{-f\left(\sigma_{k-1},\sigma_k\right)\right\}$. Then, we try the Ansatz

$$f\left(\sigma_{k-1},\sigma_k\right) = a\sigma_{k-1}\sigma_k + b\sigma_{k-1} + c\sigma_k + d.$$

This yields to the following system of equations:

$$\begin{aligned} 2\exp\left\{-\left(a+b+c+d\right)\right\} &= \exp\left\{\beta h/N\right\} + \exp\left\{-\beta h/N\right\}, \\ 2\exp\left\{-\left(-a-b+c+d\right)\right\} &= \exp\left\{\beta h/N\right\} - \exp\left\{-\beta h/N\right\}, \\ 2\exp\left\{-\left(-a+b-c+d\right)\right\} &= \exp\left\{\beta h/N\right\} - \exp\left\{-\beta h/N\right\}, \\ 2\exp\left\{-\left(a-b-c+d\right)\right\} &= \exp\left\{\beta h/N\right\} + \exp\left\{-\beta h/N\right\}, \end{aligned}$$

which solution is trivially obtained:

$$a = -\frac{1}{2}\ln\left(\coth\frac{\beta h}{N}\right); \quad b = c = 0, \quad d = -\frac{1}{2}\ln\left(\frac{1}{2}\sinh\frac{2\beta h}{N}\right).$$

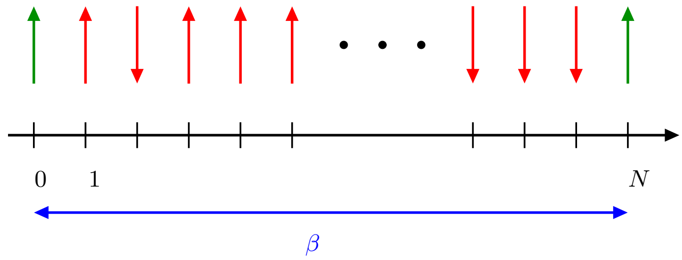

Figure 4: Schematics of a single path in the imaginary-time direction of length β with periodic boundary conditions. Equivalently, this path corresponds to a single configuration of the classical Ising chain.

Moreover, notice that $\sigma_k\sigma_{k-1} = 1 - (\sigma_k - \sigma_{k-1})^2/2$, then we rewrite

$$f(\sigma_{k-1}, \sigma_k) = a + d - \frac{a}{2}(\sigma_k - \sigma_{k-1})^2 = -\ln\left(\cosh\frac{\beta h}{N}\right) + \frac{1}{4}\ln\left(\coth\frac{\beta h}{N}\right)(\sigma_k - \sigma_{k-1})^2 .$$

Finally, we now can path integral representation of the partition function as

$$Z = \lim_{N\to\infty}\left(\cosh\frac{\beta h}{N}\right)^N \sum_{\sigma_1,\ldots,\sigma_N} e^{-S_E},$$

with

$$\begin{aligned} S_E &= \sum_{k=1}^{N}\left\{-\frac{\beta}{N}B\sigma_k + \frac{1}{4}\ln\left(\coth\frac{\beta h}{N}\right)(\sigma_k - \sigma_{k-1})^2\right\} \\ &= \sum_{k=1}^{N}\left\{-\tilde{B}\sigma_k - J\sigma_k\sigma_{k-1}\right\} + \frac{N}{2}\ln\left(\coth\frac{\beta h}{N}\right), \end{aligned} \tag{30}$$

with $J = \frac{1}{2}\ln\left(\coth\frac{\beta h}{N}\right)$ and $\tilde{B} = \frac{\beta}{N}B$. We have arrived at an important conclusion. The quantum Hamiltonian (21) thus maps to a classical Hamiltonian (30). This is the classical Hamiltonian of a classical ferromagnetic Ising chain with periodic boundary conditions $\sigma_0 = \sigma_N$ (see Fig. 4). In this classical system, we have that $\beta_{\text{cl}}J_{\text{cl}} = J$ and $\beta_{\text{cl}}B_{\text{cl}} = \tilde{B}$. We would like to call the attention to the fact that J_{cl} depends on h. For $h \to 0$, notice that $\beta_{\text{cl}}J_{\text{cl}} \to \infty$. This favors configurations that are mostly ferromagnetic, i.e., configurations in which the spins are mostly aligned. This corresponds to paths in the imaginary-time direction without spin flips. This is in accordance with the fact that quantum fluctuations are induced by $h\hat{\sigma}^x$.

The partition function is

$$Z = \lim_{N\to\infty}\left(\cosh\frac{\beta h}{N}\right)^N \sum_{\sigma_1,\ldots,\sigma_N} e^{-S_E}.$$

The one-dimensional Ising chain is well-known. Using the transfer matrix technique, we compute

$$\begin{aligned} Z &= \lim_{N\to\infty}\left(\frac{1}{2}\sinh\frac{2\beta h}{N}\right)^{\frac{N}{2}} \sum_{\sigma_1,\ldots,\sigma_N}\left\{\left[e^{J\sigma_1\sigma_2+\tilde{B}(\sigma_1+\sigma_2)/2}\right]\left[e^{J\sigma_2\sigma_3+\tilde{B}(\sigma_2+\sigma_3)/2}\right]\ldots\left[e^{J\sigma_N\sigma_1+\tilde{B}(\sigma_N+\sigma_1)/2}\right]\right\}, \\ &= \lim_{N\to\infty}\left(\frac{1}{2}\sinh\frac{2\beta h}{N}\right)^{\frac{N}{2}} \text{tr}\left\{\mathbb{T}_1\mathbb{T}_2\ldots\mathbb{T}_N\right\}, \end{aligned}$$

where

$$\mathbb{T} = \mathbb{T}_i = \begin{pmatrix} e^{J+\tilde{B}} & e^{-J} \\ e^{-J} & e^{J-\tilde{B}} \end{pmatrix}, \Rightarrow Z = \lim_{N\to\infty}\left(\cosh\frac{\beta h}{N}\right)^N \text{tr}\left\{\mathbb{T}^N\right\},$$

yielding

$$Z = \lim_{N\to\infty}\left(\frac{1}{2}\sinh\frac{2\beta h}{N}\right)^{\frac{N}{2}}\left(t_+^N + t_-^N\right), \text{ with } t_\pm = e^J\left(\cosh\tilde{B} \pm \sqrt{\sinh^2\tilde{B} + e^{-4J}}\right),$$

being the eigenvalues of $\mathbb{T}$. Note that Z will be dominated by the largest t in the limit $N \to \infty$. In this limit, $t_\pm = \sqrt{\frac{N}{h\beta}}\left[1 \pm \frac{h_{\rm tot}\beta}{N} + \mathcal{O}\left(\frac{\beta}{N}\right)^2\right]$. Then

$$\begin{aligned} Z &= \lim_{N\to\infty}\left(\frac{1}{2}\sinh\frac{2\beta h}{N}\right)^{\frac{N}{2}}\left(\sqrt{\frac{N}{h\beta}}\right)^N\left(\left(1+\frac{h_{\rm tot}\beta}{N}\right)^N + \left(1-\frac{h_{\rm tot}\beta}{N}\right)^N\right) \\ &= \left(e^{\beta h_{\rm tot}} + e^{-\beta h_{\rm tot}}\right) = 2\cosh\beta h_{\rm tot}, \end{aligned}$$

which recovers (22). From this, the thermodynamical observables follows straightforwardly.

However, it is useful to consider the $\beta \to \infty$ limit from the start. In this case, we take $\epsilon = \frac{\beta}{N}$ finite. Only in the end of the calculation we take $\epsilon \to 0$. In this case, the free-particle per particle becomes

$$f = \frac{1}{N}\left(-\ln Z\right) = -\ln t_+ + \text{const.}$$

We now can compute the magnetization

$$m = -\frac{\partial}{\partial H} f = \frac{\sinh\tilde{B}}{\sqrt{\sinh^2\tilde{B} + e^{-4J}}} = \frac{\sinh\epsilon B}{\sqrt{\sinh^2\epsilon B + \tanh^2\epsilon h}}. \tag{31}$$

Now taking the limit $\epsilon \to 0$,

$$m \to \frac{\epsilon B}{\sqrt{(\epsilon B)^2 + (\epsilon h)^2}} = \frac{h}{h_{\rm tot}}, \tag{32}$$

recovering the quantum result (24) in the limit $T \to 0$. In the same way,

$$\chi = \left.\frac{\partial}{\partial h} m\right|_{m\to 0} = \lim_{h\to 0}\frac{\epsilon}{\coth^2\epsilon h} \times \frac{1}{\left[1 + \left(\frac{1}{\sinh\epsilon B\coth\epsilon h}\right)^2\right]^{3/2}} \times \frac{1}{\sinh^3\epsilon B} = \epsilon\coth\epsilon h. \tag{33}$$

Taking the limit $\epsilon \to 0$,

$$\chi \to \epsilon \times \frac{1}{\epsilon h} = \frac{1}{h}, \tag{34}$$

which recovers the quantum result (26) at $T = 0$.

The correlation function can be computed through

$$\langle\sigma_i\sigma_{i+r}\rangle = \frac{1}{Z}\text{tr}\left\{\mathbb{T}^{i-1}\hat{\sigma}_i\mathbb{T}^r\hat{\sigma}_{i+r}\mathbb{T}^{N-i-r+1}\right\} = \frac{1}{Z}\text{tr}\left\{\hat{\sigma}_i\mathbb{T}^r\hat{\sigma}_{i+r}\mathbb{T}^{N-r}\right\}.$$

The matrix $\hat{\sigma}$ is diagonal and equals the $\hat{\sigma}^z$ Pauli matrix. We, however, wish to write it in the basis that diagonalizes $\mathbb{T}$: $\mathbb{V}^{-1}\mathbb{T}\mathbb{V} = \mathbb{D}$, where $\mathbb{V}$ is the matrix of the eigenvectors of $\mathbb{T}$:

$$\langle\sigma_i\sigma_{i+r}\rangle = \frac{1}{Z}\text{tr}\left\{\hat{\sigma}_i\mathbb{V}\mathbb{D}^r\mathbb{V}^T\hat{\sigma}_{i+r}\mathbb{V}\mathbb{D}^{N-r}\mathbb{V}^T\right\} = \frac{1}{Z}\text{tr}\left\{\begin{pmatrix} a & b \\ b & -a\end{pmatrix}\begin{pmatrix} t_+^r & 0 \\ 0 & t_-^r\end{pmatrix}\begin{pmatrix} a & b \\ b & -a\end{pmatrix}\begin{pmatrix} t_+^{N-r} & 0 \\ 0 & t_-^{N-r}\end{pmatrix}\right\},$$

with

$$\begin{pmatrix} a & b \\ b & -a\end{pmatrix} = \mathbb{V}^{-1}\hat{\sigma}^z\mathbb{V}. \text{ Since } \mathbb{V} = \begin{pmatrix} a_1 & -a_2 \\ a_2 & a_1\end{pmatrix}, \Rightarrow a = a_1^2 - a_2^2 \text{ and } b = -2a_1a_2.$$

[Note $\begin{pmatrix} a_1 \\ a_2\end{pmatrix}$ is the eigenvector with the greatest eigenvalue (t_+).] Then,

$$\begin{aligned} \langle\sigma_i\sigma_{i+r}\rangle &= \frac{1}{Z}\text{tr}\begin{pmatrix} at_+^r & bt_-^r \\ bt_+^r & -at_-^r\end{pmatrix}\begin{pmatrix} at_+^{N-r} & bt_-^{N-r} \\ bt_+^{N-r} & -at_-^{N-r}\end{pmatrix} = \frac{1}{Z}\text{tr}\begin{pmatrix} a^2t_+^N + b^2t_+^{N-r}t_-^r & ab\left(t_+^r t_-^{N-r} - t_-^N\right) \\ ab\left(t_+^N - t_+^{N-r}t_-^r\right) & b^2t_+^r t_-^{N-r} + a^2t_-^N\end{pmatrix}, \\ &= \frac{1}{t_+^N + t_-^N}\left[a^2\left(t_+^N + t_-^N\right) + b^2\left(t_+^{N-r}t_-^r + t_+^r t_-^{N-r}\right)\right] \to \frac{1}{t_1^N}\left[a^2\left(t_1^N + t_2^N\right) + b^2\left(t_1^{N-r}t_2^r + t_1^r t_2^{N-r}\right)\right], \\ &\to a^2 + b^2\left(\frac{t_-}{t_+}\right)^r + \mathcal{O}\left(\frac{t_-}{t_+}\right)^{N-r} + \mathcal{O}\left(\frac{t_-}{t_+}\right)^N, \end{aligned}$$

in the limit $N \gg r$ and $N \to \infty$.

The connected correlation function is

$$G(r) = \langle \sigma_i \sigma_{i+r} \rangle - \langle \sigma_i \rangle \langle \sigma_{i+r} \rangle .$$

Therefore, we need to compute $\langle \sigma_i \rangle$ (which equals m):

$$\begin{aligned} \langle \sigma_i \rangle &= \frac{1}{Z} \mathrm{tr} \left\{ \mathbb{T}^{i-1} \sigma_i \mathbb{T}^{N-i} \right\} = \frac{1}{Z} \mathrm{tr} \left\{ \sigma_i \mathbb{T}^N \right\} = \frac{1}{Z} \mathrm{tr} \left\{ \begin{pmatrix} a & b \\ b & -a \end{pmatrix} \begin{pmatrix} t_+^N & 0 \\ 0 & t_-^N \end{pmatrix} \right\}, \\ &= \frac{a}{t_+^N + t_-^N} \left(t_+^N - t_-^N \right) \to a. \end{aligned}$$

Finally,

$$G(r) \to a^2 + b^2 \left(\frac{t_-}{t_+} \right)^r - a^2 = b^2 e^{-r/\xi}, \text{ with } \xi = \frac{1}{\ln (t_+/t_-)}.$$

For $B = 0$, the correlation length becomes

$$\begin{aligned} \xi(B=0) &= \frac{1}{\ln \left(\left(e^J + e^{-J} \right) / \left(e^J - e^{-J} \right) \right)} = \frac{1}{\ln \left(\left(1 + e^{-2J} \right) \left(1 - e^{-2J} \right)^{-1} \right)}, \\ &\approx \frac{1}{\ln \left(\left(1 + e^{-2J} \right) \left(1 + e^{-2J} \right) \right)} = \frac{1}{2 \ln \left(1 + e^{-2J} \right)} \approx \frac{1}{2} e^{2J}, \end{aligned} \tag{35}$$

for $J \gg 1$.

Since $m = \langle \sigma_i \rangle$, it implies that

$$a = m = \frac{\sinh H}{\sqrt{\sinh^2 H + e^{-4J}}}.$$

Therefore, using the normalization of the eigenvectors ($a_1^2 + a_2^2 = 1$), we can find that $a_1^2 = (1+m)/2$. The constant

$$b^2 = (-2a_1 a_2)^2 = 4a_1^2 \left(1 - a_1^2 \right) = 4 \left(\frac{1+m}{2} \right) \left(\frac{1-m}{2} \right) = 1 - m^2 = \frac{e^{-4J}}{\sinh^2 H + e^{-4J}}.$$

Note that $b \to 0$ when $J \to \infty$, which is equivalent to $\epsilon h \to 0$ (remember that $J = \ln(\coth \epsilon h)/2$). However, when $\tilde{B} \to 0$, then $b \to 1$. Taking the $\epsilon \to 0$ limit first,

$$b \to \frac{e^{\ln(\epsilon h)^2}}{(\epsilon B)^2 + e^{\ln(\epsilon h)^2}} \to \frac{h^2}{h_{\mathrm{tot}}^2},$$

which allow us to conclude that b does not depend on ϵ. Now we can compute b in the limit $B \to 0$,

$$b = \frac{h^2}{h^2 + B^2} \to 1. \text{ Also, } \xi \to \frac{1}{2} e^{\ln(\epsilon h)^{-1}} = \frac{1}{2\epsilon h}. \tag{36}$$

Then,

$$G(r) \to \left(\frac{h^2}{h_{\mathrm{tot}}^2} \right) e^{-2\epsilon h r} = e^{-2\epsilon h r},$$

which is the same as in the quantum version (29) if we identify

$$\frac{\beta}{N} r = \frac{\tau}{\hbar}. \tag{37}$$

This confirm the proper order of taking the limits: first take $N \to \infty$ and then $\epsilon \to 0$ as the last step. Finally, this is an important result because it tells us how to relate the imaginary-time length τ (of the quantum formulation) with the real space r (of the classical formulation).

C. Generalization to higher dimensions

We now want to explicitly show that the transverse field Ising model maps to a classical Ising model in $d+1$ dimensions at $T=0$. The quantum Hamiltonian is

$$\hat{H} = -\sum_{\alpha,\beta} J_{\alpha,\beta}\hat{\sigma}^z_\alpha\hat{\sigma}^z_\beta - \sum_\alpha \left(h_\alpha\hat{\sigma}^x_\alpha + B_\alpha\hat{\sigma}^z_\alpha\right).$$

The corresponding partition function is

$$\begin{aligned} Z &= \sum_{\sigma_1,\ldots,\sigma_N} \left\langle \sigma_1,\ldots,\sigma_N \left| e^{-\beta\hat{H}} \right| \sigma_1,\ldots,\sigma_N \right\rangle = \sum_{\{\sigma_\alpha\}} \left\langle \{\sigma_\alpha\} \left| e^{-\beta\hat{H}} \right| \{\sigma_\alpha\} \right\rangle \\ &= \lim_{N\to\infty} \sum_{\{\sigma_{\alpha,0}\}} \cdots \sum_{\{\sigma_{\alpha,N}\}} \left\langle \{\sigma_{\alpha,0}\} \left| e^{-\frac{\beta}{N}\hat{H}} \right| \{\sigma_{\alpha,1}\} \right\rangle \ldots \left\langle \{\sigma_{\alpha,N-1}\} \left| e^{-\frac{\beta}{N}\hat{H}} \right| \{\sigma_{\alpha,N}\} \right\rangle. \end{aligned}$$

Then, we have to deal with the time slice

$$\begin{aligned} \left\langle \{\sigma_{\alpha,k-1}\} \left| e^{-\frac{\beta}{N}\hat{H}} \right| \{\sigma_{\alpha,k}\} \right\rangle &= \left\langle \{\sigma_{\alpha,k-1}\} \left| e^{\frac{\beta}{N}\sum_\alpha h_\alpha\hat{\sigma}^x_\alpha} e^{\frac{\beta}{N}\left(\sum_{\alpha,\gamma} J_{\alpha,\gamma}\hat{\sigma}^z_\alpha\hat{\sigma}^z_\gamma + \sum_\alpha B_\alpha\hat{\sigma}^z_\alpha\right)} \right| \{\sigma_{\alpha,k}\} \right\rangle \\ &= \left\langle \{\sigma_{\alpha,k-1}\} \left| e^{\frac{\beta}{N}\sum_\alpha h_\alpha\hat{\sigma}^x_\alpha} \right| \{\sigma_{\alpha,k}\} \right\rangle e^{\frac{\beta}{N}\left(\sum_{\alpha,\gamma} J_{\alpha,\gamma}\sigma_{\alpha,k}\sigma_{\gamma,k} + \sum_\alpha B_\alpha\sigma_{\alpha,k}\right)}. \end{aligned}$$

As in the single-spin case, the non-commuting $\hat{\sigma}^x$ term yields to

$$\left\langle \{\sigma_{\alpha,k-1}\} \left| e^{\frac{\beta}{N}\sum_\alpha h_\alpha\hat{\sigma}^x_\alpha} \right| \{\sigma_{\alpha,k}\} \right\rangle = e^{\frac{\beta}{N}\left(\sum_\alpha \frac{1}{2}\ln\left(\coth\frac{\beta h_\alpha}{N}\right)\sigma_{\alpha,k}\sigma_{\alpha,k-1} + \frac{1}{2}\ln\left(\frac{1}{2}\sinh\frac{2\beta h}{N}\right)\right)}.$$

Thus, collecting all the terms, we arrive at the Euclidean action

$$S_E = -\sum_{\alpha,\gamma,k} \tilde{J}_{\alpha,\gamma}\sigma_{\alpha,k}\sigma_{\beta,k} - \sum_{\alpha,k}\tilde{B}_\alpha\sigma_{\alpha,k} - \sum_{\alpha,k}\tilde{J}'_\alpha\sigma_{\alpha,k}\sigma_{\alpha,k-1},$$

where $\tilde{J}_{\alpha,\gamma} = \frac{\beta}{N}J_{\alpha,\gamma}$, $\tilde{B}_\alpha = \frac{\beta}{N}B_\alpha$, and $\tilde{J}'_\alpha = \frac{\beta}{2N}\ln\left(\coth\frac{\beta h_\alpha}{N}\right)$. This action corresponds to classical Ising model in $d+1$ dimensions where the coupling between the spins in the spatial dimension are $\tilde{J}_{\alpha,\gamma}$ and the couplings between the spins along the imaginary-time dimension is $\tilde{J}'_\alpha$, which are uniform along that direction (see Fig. 5).

VII. TUNNELING AND INSTANTONS

In this section, we would like to illustrate a well-known phenomenon in the path-integral representation: the quantum tunneling. We will not be able to solve the problem in full glory because of some functionals that are cumbersome to compute. However, it does not mean we cannot analyze the structure of the tunneling phenomena in the path-integral formalism. As we will show, we will be able to understand an important structure called instanton.

Consider for instance the case of a single particle in a double-well potential at zero-temperature, i.e., in its ground state (blue solid curve in Fig. 6). For simplicity, let us consider that this potential is symmetric, i.e., $V(x) = -V(x)$. We are interested in computing the (transition amplitudes) propagators $G(\pm a, \pm a, t)$, meaning the particle is originally at the left (or right) well $x_0 = \mp a$ at $t_0 = 0$ and at the right (or left) well $x_f = \pm a$ at time $t_f = t$. The particle goes from the left to the right well via quantum tunneling. Notice that a single tunneling is not the only possibility. There are many possibles tunnelings back and forth between the wells.

The propagator is a good quantity to study here because, for long times, it will probe the tunneling phenomena via the two lowest-energy Eigenstates of the problem (which are the symmetric and anti-symmetric combinations of the orbitals localized in each minima). Thus, from the structure of the propagator, namely $G \propto e^{-\frac{i}{\hbar}E_0 t} \pm ee^{-\frac{i}{\hbar}(E_0+\Delta E)t}$, we will be able to extract the energy difference between these states, and therefore, the tunneling rate at long times.

As we have learned from the path integral formulation, the particle goes from one well to the other via all possible paths. In the semiclassical approximation, we have also learned that the classical path (i.e., the one determined by classical mechanics) is the one that contributes the most. But for the quantum tunneling phenomena, notice there is no such classical path. Well, there is no such classical path in the *real* time. Recall that in the imaginary time formalism, the particle is under the influence of the inverted potential $-V(x)$ (red dashed curve in Fig. 6). In this

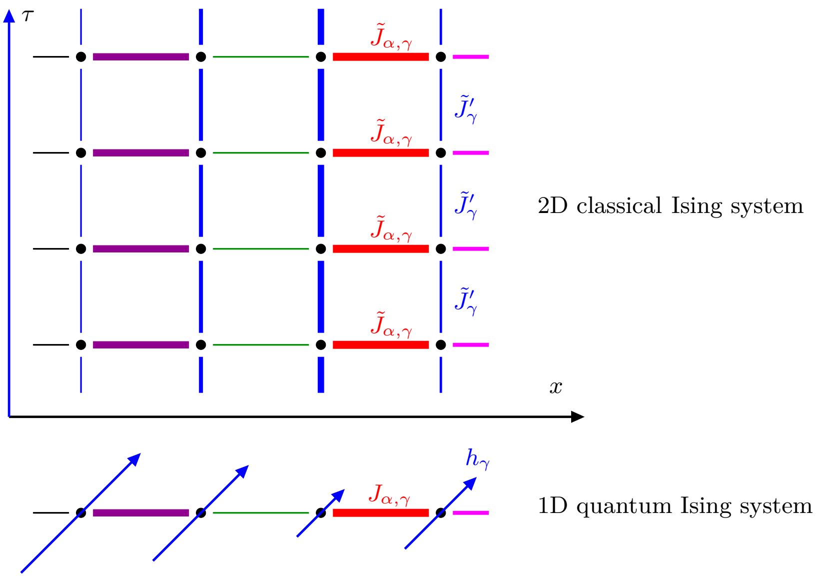

Figure 5: Schematics of a 1D quantum Ising chain mapped to a 2D classical Ising system. The vertical direction is the imaginary-time direction. Edges with different colors and thickness represent Ising couplings of different magnitudes. Likewise, arrows represent transverse fields.

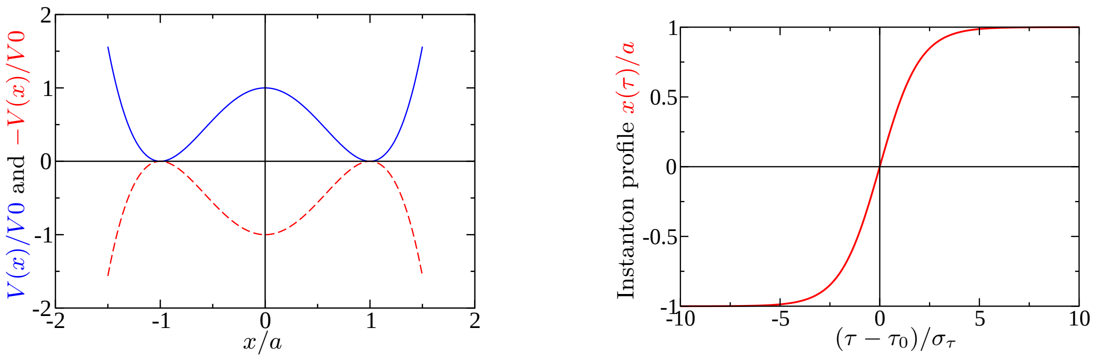

Figure 6: (Left) A symmetric double-well potential. The minima are at $x = \pm a$, and the barrier height is V_0. The red dashed curve represents the inverted potential. (Right) The corresponding instanton solution.

case, a zero-energy particle initially located at $x_0 = -a$ could propagate "downhill" until $x = 0$ and then "climb" it until $x_f = +a$. Therefore, it is natural (i.e., more intuitive [5]) to tackle this problem in the imaginary-time formalism. We then change gears and focus on the Euclidean propagators

$$\hbar\mathcal{G}\left(\pm a, \hbar\beta, \pm a, 0\right) = \int \mathcal{D}\left[x(\tau)\right] e^{-\frac{1}{\hbar}S_E}, \text{ with } S_E = \int_0^{\hbar\beta} \mathrm{d}\tau \left(\frac{1}{2}m\dot{x}^2 + V(x)\right),$$

where x is a function of the imaginary time τ. The classical stationary phase (or saddle point) path is given by $m\ddot{x}_{\rm cl} = V'(x_{\rm cl})$. For the total energy $E = 0$ case, there are two type of solutions: (a) the trivial solutions $x_{\rm cl} = \mp a$ meaning the particle stays at rest, and the interesting solutions (b) in which the particle leaves its equilibrium position $x_0 = \mp a$, pass through the "potential" minimum at $x = 0$, and finally reaches its new equilibrium position $x_f = \pm a$.

The trivial solutions (a) gives us the physics zero-point fluctuation in a single well similar to that of Eq. (20). Setting $x_0 = 0$ in Eq. (20), taking the $\beta\hbar\omega \gg 1$ limit, and Wick rotating $\beta \to it/\hbar$, we find that $i\hbar G(a, a, t) \to Fe^{-\frac{1}{\hbar}S_E[x_{\rm cl}]} = \sqrt{\frac{m\omega}{2\pi\hbar\sinh\beta\hbar\omega}}e^0 \to \sqrt{\frac{m\omega}{\pi\hbar}}e^{-\frac{1}{2}\beta\hbar\omega} \to \sqrt{\frac{m\omega}{\pi\hbar}}e^{-\frac{i}{2}\omega t}$. Notice this is a way of obtaining the Harmonic Oscillator ground-state energy since $i\hbar G \to |\phi_0(0)|^2\, e^{-\frac{i}{\hbar}E_0 t} = \sqrt{\frac{m\omega}{\pi\hbar}}e^{-\frac{i}{2}\omega t}$ in the long-time limit. Evidently, the frequency ω is obtained by $V''(\pm a) = \frac{8V_0}{a^2} = m\omega^2$.

The interesting solutions (b) is the new deal. They are called instanton solutions. In order to have a better feeling of what they are, let us try to compute these solutions. The corresponding action is

$$S_{E,\text{cl}}^{\text{inst}} = \int \mathrm{d}\tau \left(\frac{1}{2}m\dot{x}_{\text{cl}}^2 + V(x_{\text{cl}})\right) = \int \mathrm{d}\tau m\dot{x}_{\text{cl}}^2 = \int_{-a}^{a} \mathrm{d}x_{\text{cl}}\sqrt{2mV(x_{\text{cl}})},$$

where we have used that the total energy $E_E \equiv \frac{m}{2}\dot{x}^2 - V(x) = 0$. (Recall the particle actually moves in the inverted potential. Likewise, we could simply recall that the total energy is $-\frac{1}{2}m\dot{x}^2 + V(x)$.) Notice therefore that, for a generic $V(x)$, we cannot perform this integration. For that reason, let us then restrict ourselves to the potential $V(x) = V_0((x/a)^2 - 1)^2$. In this case, we can solve the classical path via the energy method: $\int_{-a}^{x_{\text{cl}}} \mathrm{d}x\sqrt{\frac{m}{2V(x)}} = \sqrt{\frac{m}{2V_0}}\int_{-1}^{x_{\text{cl}}/a}\frac{\mathrm{d}z}{1-z^2} = a\sqrt{\frac{m}{8V_0}}\ln\left(\frac{1+z}{1-z}\right)\Big|_{z=-1+0^+}^{z=x_{\text{cl}}/a} = \tau - \tau_0$. Evidently, we need to set the initial condition that at $\tau = -\infty$ the particle is at $x = -a + 0^+$, otherwise the classical particle does not leave the equilibrium position $x^{\text{eq}} = -a$. Solving the algebra, we find that

$$x_{\text{cl}}^{\text{inst}}(\tau) = -a\tanh\left(\frac{1}{2}\left(\frac{\tau-\tau_0}{\sigma_\tau}\right)\right), \text{ with } \sigma_\tau = \sqrt{\frac{ma^2}{8V_0}},$$

and we have chosen τ_0 such that $x_{\text{cl}}^{\text{inst}}(\tau_0) = 0$. The interesting feature is that for only a brief time interval (of order σ_τ) the "classical" particle is not in one of its equilibrium position $\pm a$, i.e., the particle goes from one equilibrium position to the other in a instant. Thus, the name instanton. [In the jargon, it is said that instantons are localized solutions in the imaginary time; for $|\tau - \tau_0| \gg \sigma_\tau$, then $a^2 - \left(x_{\text{cl}}^{\text{inst}}\right)^2 \approx \exp(-\left|\frac{\tau-\tau_0}{\sigma_\tau}\right|)$ with σ_τ playing the role of the instanton size, i.e., the instanton exists for a short instant of length σ_τ.] The corresponding classical action is $S_{E,\text{cl}}^{\text{inst}} = \sqrt{2mV_0}a\int_{-1}^{1}\mathrm{d}z\left(1-z^2\right) = \frac{4}{3}\sqrt{2ma^2V_0}$. Finally, although these expressions are particular for the potential $V_0((x/a)^2-1)^2$, we will assume that other symmetric non pathological double-well potentials have similar instanton-like solutions, i.e., x_{cl} is at $\pm a$ except for a brief instant of order $\sigma_\tau \propto \sqrt{\frac{ma^2}{V_0}}$ and the corresponding action is $S_{E,\text{cl}}^{\text{inst}} \propto V_0\sigma_\tau$.

Evidently, there is the anti-instanton solution $x_{\text{cl}}^{\overline{\text{inst}}}(\tau) = -x_{\text{cl}}^{\text{inst}}(\tau)$ which brings the particle from the right to the left minimum. Notice that $S_{E,\text{cl}}^{\overline{\text{inst}}} = S_{E,\text{cl}}^{\text{inst}}$.

We can now compute the single-instanton propagator in the semiclassical approach

$$\hbar\mathcal{G}^{\text{inst}} = e^{-\hbar^{-1}S_{E,\text{cl}}^{\text{inst}}}F,$$

where F is [see (14)]

$$F = \lim_{N\to\infty}\left(\frac{m}{2\pi i\hbar\Delta t}\right)^{\frac{N}{2}}\sqrt{\frac{(2\pi i\hbar)^{N-1}}{\text{Det}\,(\mathbb{M})}} \to \lim_{N\to\infty}\left(\frac{m}{2\pi\hbar\Delta\tau}\right)^{\frac{N}{2}}\sqrt{\frac{(2\pi\hbar)^{N-1}}{\text{Det}\,(\mathbb{M})}}$$

where

$$\mathbb{M} = \frac{m}{\Delta\tau}\begin{pmatrix} 2 & -1 & 0 & \cdots & 0 \\ -1 & 2 & -1 & \cdots & 0 \\ 0 & -1 & 2 & \cdots & \vdots \\ \vdots & \vdots & \vdots & \ddots & -1 \\ 0 & 0 & \cdots & -1 & 2 \end{pmatrix} + \Delta\tau\begin{pmatrix} V''\left(x_{\text{cl},1}^{\text{inst}}\right) & & & & \\ & V''\left(x_{\text{cl},2}^{\text{inst}}\right) & & & \\ & & V''\left(x_{\text{cl},3}^{\text{inst}}\right) & & \\ & & & \ddots & \\ & & & & V''\left(x_{\text{cl},N-1}^{\text{inst}}\right) \end{pmatrix},$$

and $V''(x) = \frac{8V_0}{a^2}[1 - \frac{1}{2}(1-(x/a)^2)]$. We will not compute this determinant here. Simply, we will assume the value of F is known. Notice that the anti-instanton propagator is equal to the instanton propagator.

Are we done for computing the tunneling propagator? Certainly not. First, recall that τ_0 is a almost a free parameter. By changing the position τ_0 of the instanton, the total action will not change appreciably (because we are considering the case $\sigma_\tau \ll \hbar\beta$). Thus, all paths containing a single instanton shifted will interfere constructively. How do we sum over all these possible paths? The propagator via a single instanton is thus computed by summing over all possible instants τ_1 in which the instanton exists as shown in the left panel of Fig. 7:

$$\begin{aligned}\hbar\mathcal{G}^{(1)} &= \mathcal{N}\int_0^{\hbar\beta-\sigma_\tau}\mathrm{d}\tau_1\hbar\mathcal{G}(a,\hbar\beta,a,\tau_1+\sigma_\tau)\times\hbar\mathcal{G}(a,\tau_1+\sigma_\tau,-a,\tau_1)\times\hbar\mathcal{G}(-a,\tau_1,-a,0)\\ &\approx \mathcal{N}\int^{\hbar\beta-\sigma_\tau}\mathrm{d}\tau_1\sqrt{\frac{m\omega}{\pi\hbar}}e^{-\frac{1}{2}(\hbar\beta-\tau_1-\sigma_\tau)\omega}\times e^{-\hbar^{-1}S_{E,\text{cl}}^{\text{inst}}}F\times\sqrt{\frac{m\omega}{\pi\hbar}}e^{-\frac{1}{2}\tau_1\omega} \approx \hbar\beta\sqrt{\frac{m\omega}{\pi\hbar}}F\mathcal{N}\times e^{-\hbar^{-1}S_{E,\text{cl}}^{\text{inst}}}\times\sqrt{\frac{m\omega}{\pi\hbar}}e^{-\frac{1}{2}\beta\hbar\omega},\end{aligned}$$

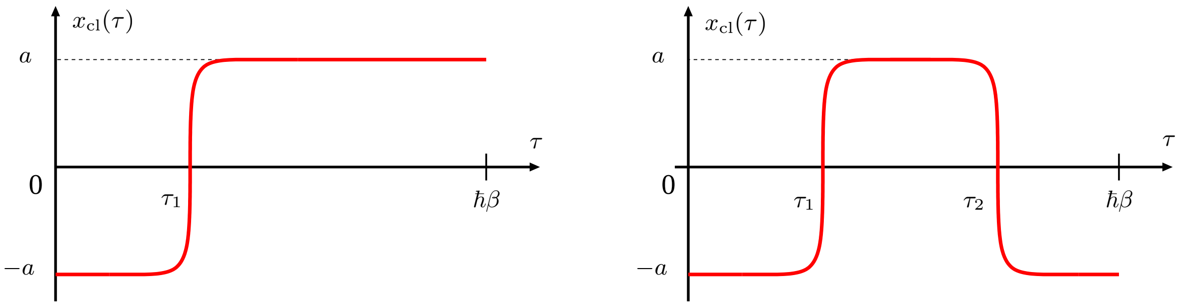

Figure 7: (Left) One instanton configuration. (Right) One instanton-anti-instanton configuration.

where $\mathcal{N}$ is a normalization constant that normalizes the integral over $\mathrm{d}\tau_1$ (and thus, absorbs the dimension of time). We will not worry about it.

How about a path containing a instanton and an anti-instanton? According to the right panel of Fig. 7, we have that

$$\begin{aligned}\hbar\mathcal{G}^{(2)} &\approx \mathcal{N}^2\int_0^{\hbar\beta}\mathrm{d}\tau_1\int_{\tau_1}^{\hbar\beta}\mathrm{d}\tau_2\sqrt{\frac{m\omega}{\pi\hbar}}e^{-\frac{1}{2}(\hbar\beta-\tau_2)\omega}\times e^{-\hbar^{-1}S_{E,\rm cl}^{\rm inst}}F\times\sqrt{\frac{m\omega}{\pi\hbar}}e^{-\frac{1}{2}(\tau_2-\tau_1)\omega}\times e^{-\hbar^{-1}S_{E,\rm cl}^{\rm inst}}F\times\sqrt{\frac{m\omega}{\pi\hbar}}e^{-\frac{1}{2}\tau_1\omega}\\ &=\frac{(\hbar\beta)^2}{2}\left(\sqrt{\frac{m\omega}{\pi\hbar}}F\mathcal{N}\right)^2\times e^{-2\hbar^{-1}S_{E,\rm cl}^{\rm inst}}\times\sqrt{\frac{m\omega}{\pi\hbar}}e^{-\frac{1}{2}\beta\hbar\omega},\end{aligned}$$

where we have to restrict $\tau_2>\tau_1$ since the instanton must come before the anti-instanton. Moreover, we are assuming that the two instantons do not interfere with each other in order to change the actual value of the action. We can justify this assumption by recalling that $\hbar\beta\gg\sigma_\tau$. Thus, there are very few configuration in which these instantons are near each other. This is called the instanton gas approximation.

It is easy to see that

$$\hbar\mathcal{G}^{(n)}=\frac{(\hbar\beta)^n}{n!}\left(\sqrt{\frac{m\omega}{\pi\hbar}}F\mathcal{N}\right)^n\times e^{-\frac{n}{\hbar}S_{E,\rm cl}^{\rm inst}}\times\sqrt{\frac{m\omega}{\pi\hbar}}e^{-\frac{1}{2}\beta\hbar\omega}=\frac{1}{n!}\left(\hbar\beta\tilde{F}\right)^n e^{-\frac{n}{\hbar}S_{E,\rm cl}^{\rm inst}}\times\sqrt{\frac{m\omega}{\pi\hbar}}e^{-\frac{1}{2}\beta\hbar\omega},$$

where the factor $\frac{(\hbar\beta)^n}{n!}=\int_0^{\hbar\beta}\mathrm{d}\tau_1\int_{\tau_1}^{\hbar\beta}\mathrm{d}\tau_2\ldots\int_{\tau_{n-1}}^{\hbar\beta}\mathrm{d}\tau_n$ and we have absorbed all these prefactor into $\tilde{F}=\sqrt{\frac{m\omega}{\pi\hbar}}F\mathcal{N}$.

We are now set to compute the propagators:

$$\begin{aligned}\hbar\mathcal{G}(a,\hbar\beta,a,0)&=\hbar\mathcal{G}^{(0)}+\hbar\mathcal{G}^{(2)}+\cdots=\sum_{n\text{ even}}\hbar\mathcal{G}^{(n)}=\sqrt{\frac{m\omega}{\pi\hbar}}e^{-\frac{1}{2}\beta\hbar\omega}\sum_{n\text{ even}}\frac{1}{n!}\left(\hbar\beta\tilde{F}\right)^n e^{-\frac{n}{\hbar}S_{E,\rm cl}^{\rm inst}},\\ &=\sqrt{\frac{m\omega}{\pi\hbar}}e^{-\frac{1}{2}\beta\hbar\omega}\cosh\left(\hbar\beta\tilde{F}e^{-\frac{1}{\hbar}S_{E,\rm cl}^{\rm inst}}\right),\\ \hbar\mathcal{G}(a,\hbar\beta,-a,0)&=\sum_{n\text{ even}}\hbar\mathcal{G}^{(n)}=\sqrt{\frac{m\omega}{\pi\hbar}}e^{-\frac{1}{2}\beta\hbar\omega}\sinh\left(\hbar\beta\tilde{F}e^{-\frac{1}{\hbar}S_{E,\rm cl}^{\rm inst}}\right).\end{aligned}$$

Notice the form

$$\hbar\mathcal{G}\left(a,\pm a,\beta\right)=\text{const}\times\left(e^{-\beta\left(\frac{1}{2}\hbar\omega-\frac{1}{2}\Delta E\right)}\pm e^{-\beta\left(\frac{1}{2}\hbar\omega+\frac{1}{2}\Delta E\right)}\right),$$

with

$$\Delta E=\hbar\tilde{F}e^{-\frac{1}{\hbar}S_{E,\rm cl}^{\rm inst}}. \tag{38}$$

Let us understand this result by recalling that, in the long-time regime, only the two quasi-degenerate lowest energy levels contribute for the propagator, i.e.,

$$\begin{aligned}\hbar\mathcal{G}&=\left\langle a\left|e^{-\beta\hat{H}}\right|\pm a\right\rangle=\langle a|S\rangle\langle S|\pm a\rangle e^{-\beta E_S}+\langle a|A\rangle\langle A|\pm a\rangle e^{-\beta E_A}\\ &=\psi_S(a)\,\psi_S^*(\pm a)\,e^{-\beta E_S}+\psi_A(a)\,\psi_A^*(\pm a)\,e^{-\beta E_A}=\text{const}\times\left(e^{-\beta E_S}\pm e^{-\beta E_A}\right)\end{aligned}$$

where the symmetric and anti-symmetric wavefunctions are

$$\psi_{S,A}(x) \approx \frac{1}{\sqrt{2}}\left(\psi(x-a) \pm \psi(x+a)\right).$$

Thus, the energy difference found in (38) is indeed the energy splitting between the degenerate states in each well when they are brought together.

The fact we would like to point out is that ΔE is non-perturbative in $\hbar$ (or more precisely, in $\hbar/S_{E,\mathrm{cl}}^{\mathrm{inst}}$). This means that the instanton calculation can capture non-perturbative effects and can be compared to the WKB method. However, the instanton gas approximation is a much better controlled method than WKB.

VIII. DISSIPATIVE SYSTEMS AND THE CALDEIRA-LEGGETT MODEL

In classical mechanics, dissipation is often described through a velocity dependent damping term in the equation of motion. Such phenomenological approach is no longer possible in quantum mechanics and a minimal microscopic understanding of the situation is necessary in order to arrive at an effective quantum mechanical model which includes dissipation. Following the seminal work of Caldeira and Leggett [6], the idea is to include dissipation by coupling the system of interest to its environment. In this section, we apply the path integral formalism to briefly investigate the quantum mechanical tunneling when the system is coupled to an external bath.

The Caldeira-Leggett Hamiltonian possesses three terms

$$\hat{H}_{CL} = \hat{H}_S + \hat{H}_B + \hat{H}_{SB}, \tag{39}$$

where

$$\hat{H}_S = \frac{\hat{p}^2}{2m} + V(\hat{q}), \tag{40}$$

is the system Hamiltonian. It models a particle of mass m moving in a potential V. Actually, the system degree of freedom does not have to be associated with a real particle and may be quite abstract. In fact, a substantial part of the calculations does not depend on the detailed form of $\hat{H}_S$. The key assumption of the model is that the environment is represented by a bath of N quantum harmonic oscillators

$$\hat{H}_B = \sum_{\alpha=1}^{N}\left(\frac{\hat{p}_\alpha^2}{2m_\alpha} + \frac{m_\alpha}{2}\omega_\alpha^2\hat{x}_\alpha^2\right). \tag{41}$$

For simplicity, we consider that the system-bath coupling is linear in the bath coordinates and thus

$$\hat{H}_{SB} = -\hat{q}\sum_{\alpha=1}^{N} c_\alpha \hat{x}_\alpha + \hat{q}^2\sum_{\alpha=1}^{N}\frac{c_\alpha}{2m_\alpha\omega_\alpha^2}, \tag{42}$$

where c_α is the coupling between the system and the α-th oscillator. The second term in $\hat{H}_{SB}$ is known as the counter-term and it is added to $\hat{H}_{SB}$ to guarantee that the minimum of the $\hat{H}_{CL}$ with respect to the system coordinate q it is still given by the minimum of the bare potential V.

A. Classical limit

To get a better understanding of the model, we begin by exploring its classical solution. The equations of motion for the bath degrees of freedom are given by

$$m\ddot{x}_\alpha = -\omega_\alpha^2 x_\alpha + \frac{c_\alpha}{m_\alpha}q,$$

for $\alpha = 1, \ldots, N$. These equations are precisely the equations of motion of a set of driven Harmonic oscillator, Eq. (54), with each driven force given by $f(t) = (c_\alpha/m_\alpha)\,q$. Their solution is then given by, Eq. (55),

$$x_\alpha(t) = x_\alpha(0)\cos(\omega_\alpha t) + \frac{p_\alpha(0)}{m_\alpha\omega_\alpha}\sin(\omega_\alpha t) + \frac{c_\alpha}{m_\alpha\omega_\alpha}\int_0^t ds\,\sin[\omega_\alpha(t-s)]\,q(s).$$

Therefore, as we couple the system to its environment, it transfers energy to the bath in the form of a driven force. Conversely, from the system point of view, such energy transfer will be translated as a dissipative term in its equation of motion. To confirm this picture, we write down the equation of motion for the system

$$m\ddot{q} \;=\; -\frac{\partial V}{\partial q}+\sum_{\alpha=1}^{N}c_{\alpha}x_{\alpha}-q\sum_{\alpha=1}^{N}\frac{c_{\alpha}^{2}}{m_{\alpha}\omega_{\alpha}^{2}}.$$

If we now substitute the solution $x_{\alpha}\left(t\right)$ for the bath degrees of freedom, we arrive at an effective equation for the system

$$\begin{aligned} m\ddot{q} \;=\; & -\frac{\partial V}{\partial q}+\sum_{\alpha=1}^{N}\frac{c_{\alpha}^{2}}{m_{\alpha}\omega_{\alpha}}\int_{0}^{t}ds\,\sin\left[\omega_{\alpha}\left(t-s\right)\right]q\left(s\right)-q\sum_{\alpha=1}^{N}\frac{c_{\alpha}^{2}}{m_{\alpha}\omega_{\alpha}^{2}} \\ & +\sum_{\alpha=1}^{N}c_{\alpha}\left[x_{\alpha}\left(0\right)\cos\left(\omega_{\alpha}t\right)+\frac{p_{\alpha}\left(0\right)}{m_{\alpha}\omega_{\alpha}}\sin\left(\omega_{\alpha}t\right)\right]. \end{aligned}$$

After an integration by parts, we obtain

$$m\ddot{q}+m\int_{0}^{t}ds\,\gamma\left(t-s\right)\dot{q}\left(s\right)+\frac{\partial V}{\partial q}=f\left(t\right), \tag{43}$$

where the external force $f\left(t\right)$ is given by

$$f\left(t\right)=\sum_{\alpha=1}^{N}c_{\alpha}\left[\left(x_{\alpha}\left(0\right)-\frac{c_{\alpha}}{m_{\alpha}\omega_{\alpha}^{2}}\right)\cos\left(\omega_{\alpha}t\right)+\frac{p_{\alpha}\left(0\right)}{m_{\alpha}\omega_{\alpha}}\sin\left(\omega_{\alpha}t\right)\right],$$

and the damping kernel

$$\gamma\left(t\right)=\frac{1}{m}\sum_{\alpha=1}^{N}\frac{c_{\alpha}^{2}}{m_{\alpha}\omega_{\alpha}}\cos\left(\omega_{\alpha}t\right).$$

Eq. (43) already tells us that the damping term is proportional to the velocity $\dot{q}\left(t\right)$. In general, however, the damping kernel has memory, i.e.$\gamma\left(t\right)$ is non-local, or correlated, in time.

A remarkable feature of the effective description for the system alone is that all quantities characterizing the environment may be expressed in terms of the spectral density of the bath

$$J\left(\omega\right)=\frac{\pi}{2}\sum_{\alpha=1}^{N}\frac{c_{\alpha}^{2}}{m_{\alpha}\omega_{\alpha}}\delta\left(\omega-\omega_{\alpha}\right). \tag{44}$$

Therefore, for practical calculations, it is not necessary to specify all oscillator parameters m_{α}, ω_{α} and c_{α} and it suffices to specify only the spectral density $J\left(\omega\right)$. For instance, the damping kernel can be rewritten as

$$\gamma\left(t\right)=\frac{2}{m}\int_{0}^{\infty}\frac{d\omega}{\pi}\frac{J\left(\omega\right)}{\omega}\cos\left(\omega t\right).$$

A commonly employed spectral function $J\left(\omega\right)$ is the so-called Ohmic damping

$$J\left(\omega\right)=\begin{cases}\eta\omega, & \omega<\Omega\\ 0, & \omega>\Omega\end{cases}, \tag{45}$$

where Ω is a high-energy cutoff. For this particular choice, the damping kernel takes the form

$$\gamma\left(t\right)=\frac{2}{m}\eta\int_{0}^{\infty}\frac{d\omega}{\pi}\cos\left(\omega t\right)=\frac{2}{m}\eta\delta\left(t\right),$$

where we took the limit $\Omega\rightarrow\infty$. Thus, the choice Ohmic damping renders $\gamma\left(t\right)$ memory-free and we recover familiar damping proportional to velocity in the effective equation of motion for the system

$$m\ddot{q}+\eta\dot{q}+\frac{\partial V}{\partial q}=f\left(t\right), \tag{46}$$

which is nothing but the usual Langevin equation for the Brownian motion. This also helps to clarify the usage of the term Ohmic damping for a linear in frequency spectral function, Eq. (45). In a LRC circuit, an Ohmic resistor also induces a memoryless damping in the equation of motion for the charge Q on the capacitor.

B. Quantum tunneling and dissipation

We wish to investigate the survival probability of a particle confined to a local minima at $q = a$ and coupled to an external environment

$$i\hbar G(at, a0) = \int \mathcal{D}\left[q\left(t\right)\right] e^{\frac{i}{\hbar}S_S[q]} \int \mathcal{D}\left[x_\alpha\left(t\right)\right] e^{\frac{i}{\hbar}\left(S_B[x_\alpha]+S_{SB}[q,x_\alpha]\right)},$$

where $q\left(0\right) = q\left(t\right) = a$, $S_S\left[q\right]$ is the system action, S_B is the bath action and S_{SB} is the system-bath coupling action. Although not crucial, it is convenient to study this problem in the imaginary-time formalism, as in the previous section. We then change gears and focus on the Euclidean propagators

$$\begin{aligned}
S_S &= \int_0^{\beta\hbar} d\tau \left(\frac{m}{2}\dot{q}^2 + V\left(q\right)\right), \\
S_B &= \int_0^{\beta\hbar} d\tau \sum_{\alpha=1}^{N} \frac{m_\alpha}{2}\left(\dot{x}_\alpha^2 + \omega_\alpha^2 x_\alpha^2\right), \\
S_{SB} &= \int_0^{\beta\hbar} d\tau \left(-q\sum_{\alpha=1}^{N} c_\alpha x_\alpha + q^2 \sum_{\alpha=1}^{N} \frac{c_\alpha^2}{2m_\alpha\omega_\alpha^2}\right),
\end{aligned}$$

where $\tau \in \left[0,\, \hbar\beta\right]$ and $\beta = 1/k_B T$. Taking the boundary condition of the fields $x_\alpha\left(\tau\right)$ also to be periodic on this imaginary time interval, we may conveniently expand all coordinates in Fourier series

$$\begin{aligned}
y\left(\tau\right) &= \sum_{n=-\infty}^{\infty} y\left(\omega_n\right) e^{i\omega_n\tau}, \\
y\left(\omega_n\right) &= \frac{1}{\beta\hbar}\int_0^{\hbar\beta} y\left(\tau\right) e^{-i\omega_n\tau} d\tau, \\
\int_0^{\hbar\beta} e^{-i\omega_n\tau} d\tau &= \hbar\beta\delta_{\omega_n,0},
\end{aligned}$$

where $y\left(\tau\right) = x_\alpha\left(\tau\right)$, $q\left(\tau\right)$. $\omega_n = 2\pi n/\beta\hbar$ are a set of discrete Fourier frequencies (generally known as bosonic Matsubara frequencies). Because the coordinates $x_\alpha$and q are real, we immediately get $y\left(-\omega_n\right) = y^\star\left(\omega_n\right)$. In Fourier space, each of the three terms of the action reads

$$\begin{aligned}
S_S &= m\left(\beta\hbar\right)\sum_n q^\star\left(\omega_n\right)\omega_n^2 q\left(\omega_n\right) + \int_0^{\beta\hbar} d\tau V\left(q\right), \\
S_B &= \left(\beta\hbar\right)\sum_{n,\alpha} m_\alpha x_\alpha^\star\left(\omega_n\right)\left(\omega_n^2 + \omega_\alpha^2\right) x_\alpha\left(\omega_n\right) = \mathbf{x}^\dagger \mathbb{M}\mathbf{x}, \\
S_{SB} &= -\left(\beta\hbar\right)\sum_{n,\alpha} q\left(\omega_n\right) c_\alpha x_\alpha^\star\left(\omega_n\right) + \sum_{n,\alpha} q^\star\left(\omega_n\right) q\left(\omega_n\right)\frac{\left(\beta\hbar\right)c_\alpha^2}{2m_\alpha\omega_\alpha^2} = \mathbf{x}^\dagger\mathbf{J} + S_{SB}^{CT},
\end{aligned}$$

where we defined $\mathbf{x}_{(\alpha,n)} = x_\alpha\left(\omega_n\right)$, $\mathbb{M}_{(\alpha,n),(\alpha',n')} = \left(\beta\hbar\right)m_\alpha\left(\omega_n^2 + \omega_\alpha^2\right)\delta_{\alpha,\alpha'}\delta_{n,n'}$, $\mathbf{J}_{(\alpha,n)} = -\left(\beta\hbar\right)c_\alpha q\left(\omega_n\right)$, and $S_{SB}^{CT} = \sum_{n,\alpha} q^\star\left(\omega_n\right) q\left(\omega_n\right)\frac{\left(\beta\hbar\right)c_\alpha^2}{2m_\alpha\omega_\alpha^2}$

Our next step is to integrate the bath degrees of freedom to generate an effective action S_{eff} to the system

$$\hbar\mathcal{G}(a,\hbar\beta,a,0) = \int \mathcal{D}\left[q\left(\omega_n\right)\right] e^{-\frac{1}{\hbar}S_S[q]} \int \mathcal{D}\left[x_\alpha\left(\omega_n\right)\right] e^{-\frac{1}{\hbar}\left(\mathbf{x}^\dagger\mathbb{M}\mathbf{x} + \mathbf{x}^\dagger\mathbf{J} + S_{SB}^{CT}\right)}.$$

The integrals over the bath variables are Gaussian, and we may easily perform them to get

$$\begin{aligned}
\hbar\mathcal{G}(a,\hbar\beta,a,0) &= \int \mathcal{D}\left[q\left(\omega_n\right)\right] e^{-\frac{1}{\hbar}S_S[q]} \underbrace{\sqrt{\frac{\left(2\pi\hbar\right)^N}{\mathrm{Det}\left(\mathbb{M}\right)}}}_{F} e^{-\frac{1}{\hbar}\left(-\frac{1}{2}\mathbf{J}\mathbb{M}^{-1}\mathbf{J}^\dagger + S_{SB}^{CT}\right)}, \\
&= F\int \mathcal{D}\left[q\left(\omega_n\right)\right] e^{-\frac{1}{\hbar}S_{eff}[q]}, \qquad (47)
\end{aligned}$$

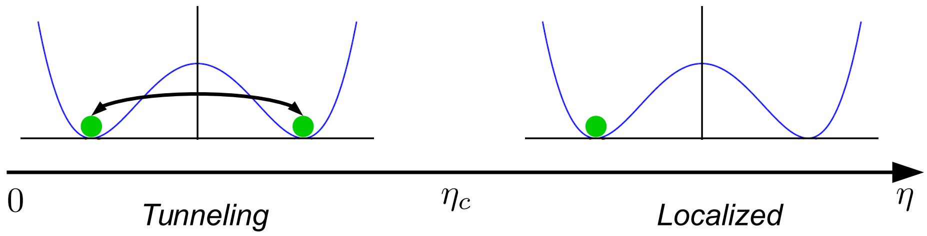

Figure 8: Caldeira-Leggett model phases as a function of the coupling to the bath.

where the effective action S_{eff} for the system is given by

$$\begin{aligned} S_{eff} &= S_S - \frac{1}{2}\mathbf{J}\mathbb{M}^{-1}\mathbf{J}^{\dagger} + S_{SB}^{CT}, \\ &= S_S - \frac{1}{2}(\beta\hbar)\sum_{n,\alpha} c_\alpha^2 \frac{q^\star(\omega_n)\,q(\omega_n)}{(\omega_n^2+\omega_\alpha^2)} + (\beta\hbar)\sum_{n,\alpha} c_\alpha^2 \frac{q^\star(\omega_n)\,q(\omega_n)}{2m_\alpha\omega_\alpha^2}, \\ &= S_S + \frac{1}{2}(\beta\hbar)\sum_{n,\alpha} \frac{c_\alpha^2\omega_n^2}{m_\alpha\omega_\alpha^2(\omega_n^2+\omega_\alpha^2)} q^\star(\omega_n)\,q(\omega_n), \\ &= S_S + \frac{1}{2}(\beta\hbar)\sum_{n,\alpha} q^\star(\omega_n)\,K(\omega_n)\,q(\omega_n), \end{aligned} \tag{48}$$

where the Kernel function $K(\omega_n)$ is defined as

$$K(\omega_n) = \frac{\omega_n^2}{\pi}\int d\omega\,\frac{J(\omega)}{\omega(\omega_n^2+\omega^2)}.$$

As in the classical solution, all information about the bath is contained in its spectral function $J(\omega)$, Eq. (44).

Therefore, by integrating out the bath degrees of freedom, the action for the system gains an induced contribution. If we now write S_{eff} in the imaginary time we have

$$S_{eff} = \int_0^{\beta\hbar} d\tau\left(\frac{m}{2}\dot{q}^2 + V(q)\right) + \int_0^{\beta\hbar} d\tau d\tau' K(\tau-\tau')\,q(\tau)\,q(\tau'),$$

which means that by interacting with the bath the quantum mechanical particle gains a self-interaction retarded in time. Moreover, the quantum Hamiltonian H_S in d dimensions maps to a classical Hamiltonian $d+1$ dimensions, with the extra dimension being the imaginary time. This is another instance of the quantum-classical mapping.

For a spectral function which shows no gap as $\omega \to 0$ the particle self-interaction will be long-ranged, or non-local, in time. To explore this long-ranged self-interaction we consider again ohmic dissipation, Eq. (45), and we get

$$K(\omega_n) = \frac{\omega_n^2}{\pi}\int d\omega\,\frac{\eta}{(\omega_n^2+\omega^2)} = \frac{\eta}{2}|\omega_n|,$$

which we now Fourier transform to obtain

$$K(\tau) = \frac{\pi\eta}{2\beta\hbar}\frac{1}{\sin^2(\pi\tau/(\beta\hbar))} \overset{\tau\ll\beta\hbar}{\simeq} \frac{\eta\beta\hbar}{2\pi}\frac{1}{\tau^2}.$$

Such non-local self-interaction of the particle has a dramatic effect on the quantum character of the particle. Consider for instance the situation where we have a double minima, as in Fig. 8. For $\eta \to 0$ we recover the usual tunneling picture discussed in the previous section and the particle tunnels back and forth among the two minima (instantons do not interact). As the coupling to the bath η increases, the particle "remembers" more and more its current position. Thus, above a critical value of coupling, dubbed the critical couplingη_c, it no longer tunnels and instead becomes localized in one of the minima. Physically we may rationalize this result as follows: tunneling is a quantum mechanical effect and as the system transfers more and more energy to the bath, the phase coherence of the particle is lost and the tunneling rate is suppressed. In the instanton language, we can say that the instantons now interact. As a last remark we stress that the precise nature of the phase transition at η_c depends on the specific form of the H_S and can be investigated in great detail by means of the quantum-classical mapping.

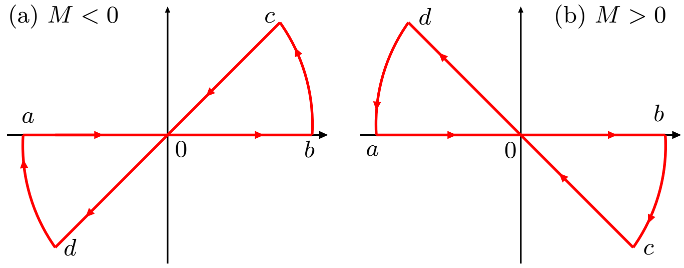

Figure 9: Integration contour in the complex plane.

IX. GAUSSIAN INTEGRALS

Gaussian integrals are usual mathematical objects in the path integral formulation of quantum mechanics. In general, we will be interested in integrals of type

$$\int \prod_{j=1}^{N} \mathrm{d}x_j e^{-\sum_{m,n} M_{m,n} x_m x_n}.$$

For the case of one single variable with real M, then we quote the well-known result

$$\int_{-\infty}^{\infty} \mathrm{d}x e^{-Mx^2} = \sqrt{\frac{\pi}{M}},$$

for $M > 0$.

For an arbitrary number of variables with $M_{m,n} = M_{n,m} \in \Re$, then we rewrite $\sum_{m,n} M_{m,n} x_m x_n = \mathbf{x}^T \mathbb{M} \mathbf{x} = \mathbf{x}^T \mathbb{V}\mathbb{D}\mathbb{V}^T \mathbf{x} = -\mathbf{y}^T \mathbb{D} \mathbf{y}$, where $\mathbb{D}_{m,n} = \lambda_m \delta_{m,m}$ is a diagonal matrix where λ_m being the Eigenvalues of $\mathbb{M}$, and $\mathbb{V}$ is a matrix whose columns $\mathbf{v}_m$ are the corresponding Eigenvectors, i.e., $\mathbb{M}\mathbf{v}_m = \lambda_m \mathbf{v}_m$. Since $\mathbb{V}\mathbb{V}^T = \mathbb{V}^T\mathbb{V} = \mathbb{I}$, then $\prod \mathrm{d}x_j = \prod \mathrm{d}y_j$. The integral then becomes

$$\int \prod \mathrm{d}x_j e^{-\mathbf{x}^T \mathbb{M} \mathbf{x}} = \int \prod \mathrm{d}y_j e^{-\sum_j \lambda_j y_j^2} = \sqrt{\prod_j \left(\frac{\pi}{\lambda_j}\right)} = \sqrt{\frac{\pi^N}{\mathrm{Det}\,(\mathbb{M})}} = \sqrt{\frac{1}{\mathrm{Det}\,(\pi^{-1}\mathbb{M})}},$$

as long as $\mathbb{M}$ is positive definite, i.e., $\lambda_m > 0$ for all m.

Let us now consider the imaginary case

$$\int \prod_{j=1}^{N} \mathrm{d}x_j e^{-i\sum_{m,n} M_{m,n} x_m x_n}.$$

Starting with the single variable case with $M \in \Re_*^-$, the integration is done via residues with the $\theta = \frac{\pi}{4}$ tilted contour sketched in Fig. 9. Thus,

$$\int_{a\to b\to c\to d\to a} e^{-iMz^2} \mathrm{d}z = 0,$$

with

$$\int_{d\to c} e^{-iMz^2} \mathrm{d}z \overset{z=xe^{i\frac{\pi}{4}}}{=} \lim_{R\to\infty} e^{i\frac{\pi}{4}} \int_{-R}^{R} e^{Mx^2} \mathrm{d}x = e^{i\frac{\pi}{4}} \sqrt{\frac{\pi}{-M}},$$

$$\int_{a\to b} e^{-iMz^2} \mathrm{d}z \overset{z=xe^{i0}}{=} \lim_{R\to\infty} \int_{-R}^{R} e^{-iMx^2} \mathrm{d}x.$$

The quarter circular integrals are vanishing. The first one reads

$$\left| \int_{b\to c} e^{-iMz^2} \mathrm{d}z \right| \overset{z=Re^{i\theta}}{=} \lim_{R\to\infty} \left| \int_0^{\frac{\pi}{4}} e^{-iMR^2(\cos 2\theta + i\sin 2\theta)} iRe^{i\theta} \mathrm{d}\theta \right| = 0,$$

for $M < 0$ because $\sin 2\theta \geq 0$ in the integration range. Likewise, the integral in the path $d \to a$ is also vanishing. Thus,

$$\int_{-\infty}^{\infty} \mathrm{d}x e^{-iMx^2} = e^{i\frac{\pi}{4}}\sqrt{\frac{\pi}{-M}} = \sqrt{\frac{\pi}{-M}e^{i\frac{\pi}{2}}} = \sqrt{\frac{\pi}{iM}}.$$

If $M > 0$, then we would have chosen the $\theta = -\frac{\pi}{4}$ tilted path instead. In this way,

$$\int_{-\infty}^{\infty} \mathrm{d}x e^{-iMx^2} = e^{-i\frac{\pi}{4}}\sqrt{\frac{\pi}{M}} = \sqrt{\frac{\pi}{M}e^{-i\frac{\pi}{2}}} = \sqrt{\frac{\pi}{iM}},$$

which is the same result as for $M < 0$.

For the case of a multiple variable imaginary Gaussian integrals, then we proceed analogously to the real case.

$$\int \prod \mathrm{d}x_j e^{-i\mathbf{x}^T \mathbb{M}\mathbf{x}} = \int \prod \mathrm{d}y_j e^{-i\sum_j \lambda_j y_j^2} = \sqrt{\prod_j \left(\frac{\pi}{i\lambda_j}\right)} = \sqrt{\frac{1}{\mathrm{Det}\left(i\pi^{-1}\mathbb{M}\right)}}.$$

Notice it can be rewritten as $e^{i(n_- - n_+)\frac{\pi}{4}} \left|\mathrm{Det}\left(\pi^{-1}\mathbb{M}\right)\right|^{-1/2}$. In this way, the phase of the integration is determined by the difference between the total number of negative n_- and positive n_+ Eigenvalues of $\mathbb{M}$.

It is also very useful to consider the Gaussian integrals with source terms:

$$\int \prod \mathrm{d}x_j e^{-\mathbf{x}^T \mathbb{M}\mathbf{x} + \mathbf{J}^T \cdot \mathbf{x}},$$

where $\mathbf{J}$ is a real vector.

This integration is easily accomplished with the previous results. For the one-variable case, we simply complete squares: $Mx^2 - Jx = M\left(x - \frac{J}{2M}\right)^2 - \frac{J^2}{4M}$. Therefore, for $M > 0$, we have that

$$\int_{-\infty}^{\infty} \mathrm{d}x e^{-Mx^2 + Jx} = \sqrt{\frac{\pi}{M}} e^{\frac{J^2}{4M}}.$$

For the multiple-variables case, we proceed similarly. Notice that $\mathbf{x}^T \mathbb{M}\mathbf{x} - \mathbf{J}^T \cdot \mathbf{x} = \mathbf{y}^T \mathbb{D}\mathbf{y} - \mathbf{J}^T \mathbb{V}\mathbf{y} = \mathbf{y}^T \mathbb{D}\mathbf{y} - \mathbf{L}^T \cdot \mathbf{y}$, with $\mathbf{y} = \mathbb{V}^T \mathbf{x}$, and $\mathbf{L} = \mathbb{V}^T \mathbf{J}$. With these results and for a positive definite $\mathbb{M}$, we have that

$$\begin{aligned}
\int \prod \mathrm{d}x_j e^{-\mathbf{x}^T \mathbb{M}\mathbf{x} + \mathbf{J}^T \cdot \mathbf{x}} &= \int \prod \mathrm{d}y_j e^{-\sum \lambda_j y_j^2 - L_j y_j} = \prod_j \sqrt{\frac{\pi}{\lambda_j}} e^{\frac{1}{4} L_j \left(\lambda_j^{-1}\right) L_j}, \\
&= \sqrt{\frac{1}{\mathrm{Det}\left(\pi^{-1}\mathbb{M}\right)}} e^{\frac{1}{4}\sum_j L_j \left(\lambda_j^{-1}\right) L_j} = \sqrt{\frac{1}{\mathrm{Det}\left(\pi^{-1}\mathbb{M}\right)}} e^{\frac{1}{4}\mathbf{L}^T \mathbb{D}^{-1}\mathbf{L}} \\
&= \sqrt{\mathrm{Det}\left(\pi \mathbb{M}^{-1}\right)} e^{\frac{1}{4}\mathbf{J}^T \mathbb{M}^{-1}\mathbf{J}},
\end{aligned}$$

where $\mathbb{I} = \mathbb{M}\mathbb{M}^{-1} = \mathbb{V}\mathbb{D}\mathbb{V}^T \mathbb{M}^{-1}$, $\Rightarrow = \mathbb{M}^{-1} = \mathbb{V}\mathbb{D}^{-1}\mathbb{V}^T$, since $\mathbb{V}^T = \mathbb{V}^{-1}$.

This result is straightforwardly generalized for the purely imaginary case:

$$\int \prod \mathrm{d}x_j e^{-i\left(\mathbf{x}^T \mathbb{M}\mathbf{x} - \mathbf{J}^T \cdot \mathbf{x}\right)} = \sqrt{\frac{1}{\mathrm{Det}\left(i\pi^{-1}\mathbb{M}\right)}} e^{\frac{i}{4}\mathbf{J}^T \mathbb{M}^{-1}\mathbf{J}}.$$

Finally, it is also interesting to compute

$$\langle x^n \rangle = \frac{\int_{-\infty}^{\infty} x^n e^{-Mx^2} \mathrm{d}x}{\int_{-\infty}^{\infty} e^{-Mx^2} \mathrm{d}x},$$

for $n \geq 0$. Notice this can be rewritten as

$$\langle x^n \rangle = \sqrt{\frac{M}{\pi}} \lim_{J \to 0} \frac{\partial^n}{\partial J^n} \int_{-\infty}^{\infty} e^{-Mx^2 + Jx} \mathrm{d}x = \lim_{J \to 0} \frac{\partial^n}{\partial J^n} \left(e^{\frac{J^2}{4M}}\right) = \frac{1}{(2M)^{\frac{n}{2}}} \times \lim_{x \to 0} \frac{\partial^n}{\partial x^n} \left(e^{\frac{1}{2}x^2}\right).$$

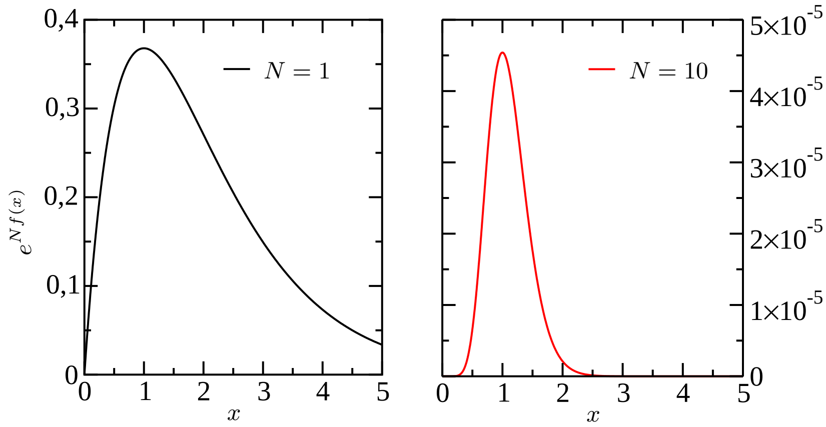

Figure 10: $e^{Nf(x)}$ for $f(x)=\ln(x)-x$ and two different values of N. The function $f(x)$ has a maximum at $x_0=1$.

Defining $k_n=\lim_{x\to 0}\frac{\partial^n}{\partial x^n}\left(e^{\frac{1}{2}x^2}\right)$, we have that $k_1=\lim_{x\to 0}\left(xe^{\frac{1}{2}x^2}\right)=0$. Likewise, it vanishes for all odd n because the integrand is an odd function. For $n=2$, we have that $k_2=\lim_{x\to 0}\left(1+x^2\right)e^{\frac{1}{2}x^2}=1$. For $n=4$, we have that $k_4=\lim_{x\to 0}\left(3+6x^2+x^4\right)e^{\frac{1}{2}x^2}=3$. For $n=6$, we have that $\left\langle x^6\right\rangle=3+12=15$. In general, $k_n=(n-1)!!$. Then

$$\left\langle x^n\right\rangle=(n-1)!!\,(2M)^{-\frac{n}{2}},$$

for n even, and $\left\langle x^n\right\rangle=0$, otherwise.

In the multiple-variable case, the n-point correlation is

$$\left\langle x_{\alpha_1}x_{\alpha_2}\ldots x_{\alpha_n}\right\rangle=\frac{\int_{-\infty}^{\infty}\prod_k \mathrm{d}x_k\left(x_{\alpha_1}x_{\alpha_2}\ldots x_{\alpha_n}e^{-\mathbf{x}^T\mathbb{M}\mathbf{x}}\right)}{\int_{-\infty}^{\infty}\prod_k \mathrm{d}x_k\left(e^{-\mathbf{x}^T\mathbb{M}\mathbf{x}}\right)},$$

where n is even and all α's indices are different from each other. This mean value is

$$\left\langle x_{\alpha_1}x_{\alpha_2}\ldots x_{\alpha_n}\right\rangle=\frac{1}{\sqrt{\mathrm{Det}\left(\pi\mathbb{M}^{-1}\right)}}\lim_{\mathbf{J}\to 0}\frac{\partial^n}{\partial J_{\alpha_1}\ldots\partial J_{\alpha_n}}\int_{-\infty}^{\infty}\prod_k \mathrm{d}x_k e^{-\mathbf{x}^T\mathbb{M}\mathbf{x}+\mathbf{J}^T\cdot\mathbf{x}}=\lim_{\mathbf{J}\to 0}\frac{\partial^n}{\partial J_{\alpha_1}\ldots\partial J_{\alpha_n}}\left(e^{\frac{1}{4}\mathbf{J}^T\mathbb{M}^{-1}\mathbf{J}}\right).$$

It is useful to analyze the small n cases. For $n=2$, we have that $\left\langle x_{\alpha_1}x_{\alpha_2}\right\rangle=\lim_{\mathbf{J}\to 0}\frac{\partial^2}{\partial J_{\alpha_1}\partial J_{\alpha_2}}\left(e^{\frac{1}{4}\mathbf{J}^T\mathbb{M}^{-1}\mathbf{J}}\right)=\left(\frac{1}{4}M^{-1}_{\alpha_1,\alpha_2}\right)$. For $n=4$, we have that $\left\langle x_{\alpha_1}\ldots x_{\alpha_4}\right\rangle=\left\langle x_{\alpha_1}x_{\alpha_2}\right\rangle\left\langle x_{\alpha_3}x_{\alpha_4}\right\rangle+\left\langle x_{\alpha_1}x_{\alpha_3}\right\rangle\left\langle x_{\alpha_2}x_{\alpha_4}\right\rangle+\left\langle x_{\alpha_1}x_{\alpha_4}\right\rangle\left\langle x_{\alpha_2}x_{\alpha_3}\right\rangle$. For an arbitrary value of even n, we simply have that

$$\left\langle x_{\alpha_1}x_{\alpha_2}\ldots x_{\alpha_n}\right\rangle=\sum_{P(\{\alpha_i\})}\left\langle x_{P(\alpha_1)}x_{P(\alpha_2)}\right\rangle\ldots\left\langle x_{P(\alpha_{n-1})}x_{P(\alpha_n)}\right\rangle,$$

which is the sum of all possible pairings. This is known as the Wick theorem for real variables.

A. Large-N methods

Suppose we want to evaluate the following integral

$$W_1=\int_a^b e^{Nf(x)},$$

in the limit where the number $N\gg 1$ for a generic function $f(x)$. If the function $f(x)$ displays a maximum at x_0, the integrand is sharply peaked around x_0 and the integral is dominated for values of x around x_0, see Fig. 10.

We then proceed by expanding $f(x)$ around its maximum x_0 up to second order

$$f(x)\approx f(x_0)-\frac{1}{2}\left|f''(x_0)\right|(x-x_0)^2,$$

and the integral W_1 may then be rewritten as

$$W_1 \approx e^{Nf(x_0)} \int_{-\infty}^{+\infty} e^{-\frac{1}{2}N\left|f''(x_0)\right|(x-x_0)^2}.$$

Because the chief contribution to $e^{Nf(x)}$ comes for x in the neighborhood of x_0, we can safely send the limits of integration to infinity, such that we are left with a Gaussian integral which we readily evaluate to get

$$W_1 \approx e^{Nf(x_0)} \sqrt{\frac{2\pi}{N\left|f''(x_0)\right|}}, \qquad N \gg 1. \tag{49}$$

We can easily extend this method to several variables, where we now consider

$$W_D = \int \prod_{i=1}^{D} dx_i e^{Nf(\vec{x})},$$

with $\vec{x} = (x_1, x_2, \ldots, x_D)$. If we apply the same steps as above, assuming again that the function $f(\vec{x})$ shows a maximum at $\vec{x} = \vec{x}_0$, we then obtain

$$W_D \approx e^{Nf(\vec{x}_0)} \sqrt{\left(\frac{2\pi}{N}\right)^D \frac{1}{\text{Det}\left(-\mathbb{H}\right)}}, \qquad N \gg 1, \tag{50}$$

where

$$\mathbb{H}_{ij} = \left.\frac{\partial^2 f}{\partial x_i \partial x_j}\right|_{\vec{x}=\vec{x}_0},$$

is the Hessian matrix evaluated at the maximum $\vec{x}_0$. Another interesting feature of this method is that in the case where $f(\vec{x})$ shows several maxima, we may simply approximate the whole integral as the sum of the individual contribution of each maximum as calculated above.

Consider now the situation where the exponent is complex (a phase), again for $N \gg 1$

$$\tilde{W}_D = \int \prod_{i=1}^{D} dx_i e^{-iNf(\vec{x})}.$$

If we now employ our generalization of Gaussian integrals for a purely imaginary exponent we then immediately obtain, see also Fig. 3,

$$\tilde{W}_D \approx e^{-iNf(\vec{x}_0)} \sqrt{\left(\frac{2\pi}{iN}\right)^D \frac{1}{\text{Det}\left(\mathbb{H}\right)}}, \qquad N \gg 1, \tag{51}$$

with the Hessian matrix defined as above. Although this result resembles very much the one for a real exponent, there is a crucial distinction: $\vec{x}_0$ no longer needs to be a maximum of $f(\vec{x}_0)$. Actually, all that is now required is that $\nabla f(x)|_{\vec{x}=\vec{x}_0} = 0$, i.e. $\vec{x}_0$ is simply an extreme of $f(\vec{x})$. Therefore, it is no surprise that the large-N method for complex exponents is sometimes referred to as saddle point or stationary phase approximation.

We close our discussion of this method by establishing the celebrated Stirling's approximation:

$$n! = n\ln n - n + \mathcal{O}(\ln n). \tag{52}$$

We begin by rewriting the factorial of n in terms of the Gamma function

$$\begin{aligned} n! &= \int_0^{\infty} x^n e^{-x} dx, \\ &= \int_0^{\infty} e^{n\left(\ln x - x/n\right)} dx, \\ &= e^{n\ln n} n \int_0^{\infty} e^{n\left(\ln y - y\right)} dy, \end{aligned}$$

where in the last line we performed a change of variables $y = x/n$. We now consider $n \gg 1$ (the integrand is depicted in Fig. 10) and from Eq. (49) we then obtain

$$n! \approx ne^{n\ln n - n}\sqrt{\frac{2\pi}{n}},$$

and thus

$$\ln n! \approx n\ln n - n + \frac{1}{2}\ln n + \frac{1}{2}\ln 2\pi. \tag{53}$$

X. DRIVEN HARMONIC OSCILLATOR

We briefly the solution of the classical driven harmonic oscillator

$$m\ddot{x} = -m\omega^2 x + f(t), \tag{54}$$

in the presence of a generic force $f(t)$. We know that the general solution for this problem can be written as

$$x(t) = x_p(t) + A\cos(\omega t) + B\sin(\omega t),$$

where $x_p(t)$ is the particular solution which depends on the specific form of the force $f(t)$. To construct a particular solution for any given force, we write $f(t)$ as

$$f(t) = \int_0^\infty f(s)\,\delta(t-s)\,ds,$$

where we assume that $f(t)$ started to act at the time $t = 0$. The key point is that Eq. (54) is linear, and thus we may solve it for a single delta function and then construct $x_p(t)$ by integrating over all possible delta functions weighted by $f(t)$. For a single delta function, Eq. (54) is given by

$$m\ddot{x}_s + m\omega^2 x_s = \delta(t)\,f(t),$$

with

$$x_s(t) = \begin{cases} 0, & t < 0 \\ A\cos(\omega t) + B\sin(\omega t), & t > 0 \end{cases}$$

because the force only acts at $t = 0$ and we assume that the oscillator was at rest for $t < 0$. Because $x_s(t)$ must be continuous at $t = 0$, since it obeys a second order differential equation, (54), we then have that $A = 0$. To fix B, we perform the usual trick when dealing with delta functions: we integrate around $t = 0$

$$\begin{aligned} m\int_{-\varepsilon}^{+\varepsilon} dt\ddot{x}_s + m\omega^2\int_{-\varepsilon}^{+\varepsilon} dt x_s &= \int_{-\varepsilon}^{+\varepsilon} dt\delta(t)\,f(t), \\ m\dot{x}_s(\varepsilon) - m\dot{x}_s(\varepsilon) + m\omega^2 x_s(0)\,2\varepsilon &= f(0), \\ m\dot{x}_s\left(0^+\right) &= f(0), \end{aligned}$$

where in the second line we considered that $x_s(0)$ is continuous at $t = 0$ and in the third line we took the limit $\varepsilon \to 0$, considering that $\dot{x}_s(0^-) = 0$ because the oscillator was at rest for $t < 0$. This equation immediately gives us that $B = f(0)/m\omega$ and we then have

$$x_s(t) = \begin{cases} 0, & t < 0 \\ (f(0)/m\omega)\sin(\omega t), & t > 0 \end{cases}$$

and thus the particular solution, $x_p(t) = \int_0^t x_s(s)\,ds$, is given by

$$x_p(t) = \int_0^t \frac{\sin[\omega(t-s)]}{m\omega} f(s)\,ds. \tag{55}$$

where $G(t-s) = \sin[\omega(t-s)]/m\omega$ is the classical Green's function, or propagator, for the harmonic oscillator.

For completeness, we compute the classical action for this system

$$S_{\rm cl} = m\int_0^t \mathrm{d}t\left(\frac{1}{2}\dot{x}_{\rm cl}^2 - \frac{1}{2}\omega^2 x_{\rm cl}^2 + f\left(t\right)x_{\rm cl}\right),$$

with the boundary conditions $x_i = x_{\rm cl}\left(0\right)$ and $x_f = x_{\rm cl}\left(t\right)$. As for the free harmonic oscillator we rewrite it as

$$S_{\rm cl} = \frac{m}{2}\left. x_{\rm cl}\dot{x}_{\rm cl}\right|_0^t + \frac{1}{2}\int_{t_i}^{t_f} f\left(t\right)x_{\rm cl}dt,$$

where we now have the extra term due to the driving force. All that is left for us to do is to fix the constants A and B in terms of the boundary conditions. After a lengthly algebra we then get [7]

$$\begin{aligned} S_{\rm cl} &= \frac{m\omega}{2\sin\left(\omega t\right)}\left[\left(x_f^2 + x_i^2\right)\cos\left(\omega t\right) - 2x_f x_i + \frac{2}{m\omega}x_f\int_0^t ds\,\sin\left[\omega s\right]f\left(s\right)\right. \\ &+ \left.\frac{2}{m\omega}x_i\int_0^t ds\,\sin\left[\omega\left(t-s\right)\right]f\left(s\right) - \frac{2}{m^2\omega^2}\int_0^t du\int_0^u ds f\left(u\right)f\left(s\right)\sin\left[\omega\left(t-u\right)\right]\sin\left[\omega s\right]\right]. \end{aligned}$$

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[1] In many occasions, the Heaviside function will not appear because it is implicit that $t > t_0$.
[2] See, for instance, the Wikipedia entry for the Baker-Campbell-Hausdorff formula.
[3] In fact, there is not need of using any of these fancy formulas. In the $\Delta t \to 0$ limit, we have from (2) that $\hat{U} = \mathbb{I} + \frac{1}{i\hbar}\Delta t\hat{H} + \mathcal{O}\left(\Delta t\right)^2$. Using this expansion up to 1st order in Δt and then re-exponentiating, we arrive at the same result that $\hat{U} \to e^{\frac{\Delta t}{i\hbar}\hat{T}}e^{\frac{\Delta t}{i\hbar}\hat{V}}$.
[4] Notice we are considering that there is only one stationary-phase path $x_{\rm cl}$. It there were more than one such path, then we have to take them into account. Provided that they are not degenerate (meaning, typically, $|x_{{\rm cl},i} - x_{{\rm cl},j}| \gg\sim \sqrt{\hbar}$), then the semiclassical result is simply the sum of many Gaussian integrals around each special path $x_{{\rm cl},k}$, i.e., $\sum_k F_k e^{\frac{i}{\hbar}S[x_{\rm cl.k}]}$.
[5] Let us be honest here, if there are classical paths, we can conveniently use the semiclassical approximation.
[6] A. O. Caldeira and A. J. Leggett, *Phys. Rev. Lett.* **46**, 211 (1981).
[7] See, for instance, this derivation.