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Bachelor Thesis

Path Integration via Infinitesimal Complex Time Phases

by

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Institute for Theoretical Condensed Matter physics (TKM)
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Contents

1 Introduction

The path integral formalism is an alternative description of quantum mechanics that is equivalent to the standard formulations which exhibits an intuitive point of view on many quantum processes. Its first complete formalisation was done by Feynman in his doctoral thesis [Feynman and Brown, 1942]. It is based on the idea that all possible paths a system can take account for the development of its quantum state – with the contribution of each path determined by its action. We give a deduction of the path integral in section 2, together with some simplifications that are possible after certain general assumptions on the system's Hamiltonian.

In classical mechanics, the equations of motion of a particle or system can be derived by finding a path in its configuration space which produces minimal action. For the quantum mechanical path integrals, though, the action becomes a complex number, demanding the search for saddle points instead of minima. We motivate the reduction of the problem to working only at the saddle point paths rather than the whole path space by giving a short introduction to the saddle point method in the case of functions with real exponents in section 3.

In certain cases, the problems arising with this complexification can be resolved by switching back and forth from real to imaginary time, where the calculation resembles a classical action minimization. This Wick rotation, which we discuss in section 4, was first introduced in [Wick, 1954] and is a useful tool for the evaluation of path integrals. However, there is little insight on the physical interpretation of this mathematical trick.

This work tries to fathom how those time rotations are justified or even necessitated by the laws of physics, with the example of a particle in a double well potential $V(x) = \kappa(x + a)^2(x - a)^2$. We regard the case of a single tunneling process in the infinite time limit. Here, the methods that suggest themselves for finding a minimal action path that connects both wells are unsuccessful when they are applied in real time. Indeed we see in section 5 that performing a Wick rotation and using these methods afterwards leads to a reasonable set of connecting paths.

Following the result of Cherman and Ünsal given in [Cherman and Ünsal, 2014], in section 7 we expound that it is not necessary to completely turn the time axis from purely real to purely imaginary in the case of the double well potential. In fact, it proves sufficient for the rotation of the time axis in the complex plane to be arbitrarily small. However, with the rotation angle approaching zero, the resulting solution paths blow up to divergingly large and spiry curves. This divergence, discussed in section 8, elucidates why the limit of null rotation can not be used.

Our idea is that the rotation emerges from fluctuations of the rest energy. In section 9, we examine how a slight complex phase of the non-zero ground state energy results in solutions that are similar to those obtained by a small rotation of the time axis. We can only make the claim plausible that complex energies give the same results as complex times by numerical comparisons; a rigorous proof of this proposition might need techniques that exceed the framework of this thesis. Then, the conceptual question would be shifted from the interpretation of imaginary times towards that of small energies with exiguous imaginary parts. The incidence of a non-zero energy is forced by basic quantum mechanical principles like Heisenberg's uncertainty principle, while the issue of explaining a complex phase of the energy is left open.

I would like to thank Jörg Schmalian for proposing the topic and supervising this bachelor thesis, Pia Gagel for her great assistance and guidance throughout this work, Tim Ludwig for bringing in many crucial ideas during our discussions, and my friends and family, especially those who did some proofreading, for their amiable support.

Logic will get you from A to Z;
imagination will get you
everywhere.

attributed to Albert Einstein

2 The Path Integral Formalism

In this first section we construct the path integral which equals the transition probability between two quantum states. This formalism was introduced by Feynman in 1965 in [Feynman and Hibbs, 1965]. A general derivation is given in [Kleinert, 1995] and [Altland and Simons, 2010].

By the laws of quantum mechanics, the probability for a point particle that is in state x_L at time t_a to be found in state x_R at a later time t_b is

$$(x_R.t_b \mid x_L.t_a) = \langle x_R | \hat{U}(t_b, t_a) | x_L \rangle \tag{1}$$

with the time evolution operator $\hat{U}(t_b, t_a)$ that is determined by the Hamiltonian of the system. We divide the time interval between t_a and t_b into a large number N of smaller intervals by introducing time steps t_n with

$$t_n - t_{n-1} = \frac{t_b - t_a}{N} =: \epsilon,\ t_0 = t_a,\ t_N = t_b. \tag{2}$$

We split up the time evolution operator accordingly, and equation 1 becomes

$$(x_R.t_b \mid x_L.t_a) = \langle x_R | \hat{U}(t_b, t_{N-1}) \cdots \hat{U}(t_{n+1}, t_n) \cdot \hat{U}(t_n, t_{n-1}) \cdots \hat{U}(t_1, t_a) | x_L \rangle . \tag{3}$$

Now between each two steps we insert the identity operator

$$1 = \int_{-\infty}^{+\infty} dx_n \, |x_n\rangle \langle x_n| \tag{4}$$

and receive

$$
\begin{aligned}
(x_R.t_b \mid x_L.t_a) &= \langle x_R|\, \hat{U}(t_b, t_{N-1}) \int_{-\infty}^{+\infty} dx_{N-1}\, |x_{N-1}\rangle \langle x_{N-1}|\, \hat{U}(t_{N-1}, t_{N-2}) \cdots |x_L\rangle \\
&= (\prod_{n=1}^{N-1} \int_{-\infty}^{+\infty} dx_n)\, \langle x_R|\, \hat{U}(t_b, t_{N-1})\, |x_{N-1}\rangle \langle x_{N-1}|\, \hat{U}(t_{N-1}, t_{N-2}) \cdots |x_L\rangle \\
&= (\prod_{n=1}^{N-1} \int_{-\infty}^{+\infty} dx_n) \prod_{n=1}^{N} (x_n.t_n \mid x_{n-1}.t_{n-1}).
\end{aligned}
\tag{5}
$$

We can write the small transition steps as

$$
(x_n.t_n \mid x_{n-1}.t_{n-1}) = \langle x_n|\, \hat{U}(t_n, t_{n-1})\, |x_{n-1}\rangle = \langle x_n|\, e^{\frac{-i}{\hbar}\epsilon \hat{H}}\, |x_{n-1}\rangle \tag{6}
$$

where we assume that the system's Hamiltonian is time-independent. Another assumption about the Hamiltonian we are using is that we can write it as

$$
\hat{H}(p, x, t) = \hat{T}(p) + \hat{V}(x), \tag{7}
$$

i.e. that it and consists of separated, time-independent kinetic and potential parts, depending solely on p respectively x. With this, the commutator $[\epsilon \hat{T}, \epsilon \hat{V}]$ is of order ϵ^2 and thus can be neglected for small ϵ . Using the Baker–Campbell–Hausdorff formula this yields:

$$
\begin{aligned}
\hat{U}(t_n, t_{n-1}) = e^{\frac{-i}{\hbar}\epsilon \hat{H}} &= e^{\frac{-i}{\hbar}\epsilon(\hat{T}+\hat{V})} \\
= e^{\frac{-i}{\hbar}\epsilon \hat{T}} e^{\frac{-i}{\hbar}\epsilon \hat{V}} (1 + \mathcal{O}(\epsilon^2)) &\approx e^{\frac{-i}{\hbar}\epsilon \hat{T}} e^{\frac{-i}{\hbar}\epsilon \hat{V}}.
\end{aligned}
\tag{8}
$$

Again inserting $1 = \int\limits_{-\infty}^{+\infty} dx \, |x\rangle \langle x|$, the single steps read

$$(x_n.t_n \mid x_{n-1}.t_{n-1}) = \langle x_n| \, e^{\frac{-i}{\hbar}\epsilon \hat{T}} e^{\frac{-i}{\hbar}\epsilon \hat{V}} \, |x_{n-1}\rangle = \int\limits_{-\infty}^{+\infty} dx \, \langle x_n| \, e^{\frac{-i}{\hbar}\epsilon \hat{T}} \, |x\rangle \langle x| \, e^{\frac{-i\epsilon \hat{V}}{\hbar}} \, |x_{n-1}\rangle \,. \tag{9}$$

As assumed, the potential energy $V(x)$ only depends on the position x, which means that the position eigenkets $|x\rangle$ are eigenkets of $\hat{V}$:

$$\hat{V} \, |x\rangle = V(x) \, |x\rangle \tag{10}$$

$$\langle x| \, e^{\frac{-i}{\hbar}\epsilon \hat{V}} \, |x_{n-1}\rangle = e^{\frac{-i}{\hbar}\epsilon V(x_{n-1})} \delta(x, x_{n-1}) \tag{11}$$

Thus equation 9 becomes

$$(x_n.t_n \mid x_{n-1}.t_{n-1}) = e^{\frac{-i}{\hbar}\epsilon V(x_{n-1})} \langle x_n| \, e^{\frac{-i}{\hbar}\epsilon \hat{T}(\hat{p})} \, |x_{n-1}\rangle \,, \tag{12}$$

and as we want to evaluate the operator $\hat{T}$ which is described in the momentum basis, we insert $1 = \int_{-\infty}^{+\infty} dp\, |p\rangle \langle p|$ and get

$$
\begin{aligned}
(x_n.t_n \mid x_{n-1}.t_{n-1}) &= e^{\frac{-i}{\hbar}\epsilon V(x_{n-1})} \langle x_n| \, e^{\frac{-i}{\hbar}\epsilon \hat{T}(\hat{p})} \int_{-\infty}^{+\infty} dp\, |p\rangle \langle p \mid x_{n-1}\rangle \\
&= \int_{-\infty}^{+\infty} dp\;\, e^{\frac{-i}{\hbar}\epsilon V(x_{n-1})} \langle x_n| \, e^{\frac{-i}{\hbar}\epsilon \hat{T}(\hat{p})} \, |p\rangle \frac{1}{\sqrt{2\pi\hbar}} e^{\frac{i}{\hbar} p x_{n-1}} \\
&= \int_{-\infty}^{+\infty} dp\;\, e^{\frac{-i}{\hbar}\epsilon V(x_{n-1})} e^{\frac{-i}{\hbar}\epsilon T(p)} \langle x_n \mid p\rangle \frac{1}{\sqrt{2\pi\hbar}} e^{\frac{-i}{\hbar} p x_{n-1}} \\
&= \int_{-\infty}^{+\infty} dp\;\, e^{\frac{-i}{\hbar}\epsilon V(x_{n-1})} e^{\frac{-i}{\hbar}\epsilon T(p)} \frac{1}{\sqrt{2\pi\hbar}} e^{\frac{i}{\hbar} p x_n} \frac{1}{\sqrt{2\pi\hbar}} e^{\frac{-i}{\hbar} p x_{n-1}} \\
&= \int_{-\infty}^{+\infty} \frac{dp}{2\pi\hbar}\; e^{\frac{-i}{\hbar}(\epsilon V(x_{n-1}) + \epsilon T(p) - p(x_n - x_{n-1}))}.
\end{aligned}
\tag{13}
$$

Now we can use that for very small $\epsilon = t_n - t_{n-1}$ the definition of the time derivative states that

$$
x_n - x_{n-1} = \epsilon \frac{x_n - x_{n-1}}{t_n - t_{n-1}} = \epsilon \dot{x}_n \tag{14}
$$

and hence we have

$$
(x_n.t_n \mid x_{n-1}.t_{n-1}) = \int_{-\infty}^{+\infty} \frac{dp}{2\pi\hbar}\; e^{\frac{-i}{\hbar}\epsilon(V(x_{n-1}) + T(p) - p\dot{x}_n)} \qquad = \int_{-\infty}^{+\infty} \frac{dp}{2\pi\hbar}\; e^{\frac{i}{\hbar}\epsilon(p\dot{x}_n - H(x_{n-1}, p))}. \tag{15}
$$

Inserting this into equation 5 gives us

$$
\begin{aligned}
(x_R.t_b \mid x_L.t_a) &= \left(\prod_{n=1}^{N-1}\int_{-\infty}^{+\infty} dx_n\right)\prod_{n=1}^{N}\left(\int_{-\infty}^{+\infty}\frac{dp_n}{2\pi\hbar}\ e^{\frac{i}{\hbar}\epsilon(p_n\dot{x}_n - H(x_{n-1},p_n))}\right) \\
&= \left(\prod_{n=1}^{N-1}\int_{-\infty}^{+\infty} dx_n\right)\left(\prod_{n=1}^{N}\int_{-\infty}^{+\infty}\frac{dp_n}{2\pi\hbar}\right)\ e^{\sum_{n=1}^{N}\frac{i}{\hbar}\epsilon(p_n\dot{x}_n - H(x_{n-1},p_n))}.
\end{aligned}
\tag{16}
$$

Using the dependency of x_{n-1}, $\dot{x}_n$ and p_n of the counting parameter n in

$$\sum_{n=1}^{N}\frac{i}{\hbar}\epsilon\left(p_n\dot{x}_n - H(x_{n-1},p_n)\right) \tag{17}$$

we make functions of the time $t_n = t_a + n\epsilon$:

$$\sum_{n=1}^{N}\frac{i}{\hbar}\epsilon\left(p(t_n)\dot{x}(t_n) - H(x(t_n),p(t_n))\right). \tag{18}$$

The sum 18 is a Riemann sum, and therefore, for small ϵ it converges to the integral

$$\int_{t_a}^{t_b}\frac{i}{\hbar}dt\left(p\dot{x} - H(x,p)\right). \tag{19}$$

Also, for this point of view of x, $\dot{x}$ and p depending on t, the functions $x(t)$ and $p(t)$ themselves are becoming the integration variables in 16; for the limit $N \to \infty$, we write

$$\left(\prod_{n=1}^{N-1}\int_{-\infty}^{+\infty} dx_n\right)\left(\prod_{n=1}^{N}\int_{-\infty}^{+\infty}\frac{dp_n}{2\pi\hbar}\right) =: \int\int\frac{\mathcal{D}x\mathcal{D}p}{2\pi\hbar}. \tag{20}$$

This means we integrate over all smooth functions $x(t)$ with $x(t_a) = x_L$ and $x(t_b) = x_R$

and smooth functions $p(t)$ with $p(t_a) = 0$.

Putting this together, equation 16 becomes

$$(x_R.t_b \mid x_L.t_a) = \int\int \frac{\mathcal{D}x\mathcal{D}p}{2\pi\hbar}\; e^{\frac{i}{\hbar}\int_{t_a}^{t_b} dt(p\dot{x}-H(x,p))}. \tag{21}$$

That is the path integral formulation of the transition probability.

Simplification of this expression can be attained if we assume that the kinetic energy is of the form of that of a point particle,

$$T(p) = \frac{p^2}{2m}. \tag{22}$$

We go back to the notation as in 15 by replacing the path integral notation by what it precisely stands for and thus have

$$\begin{aligned}
(x_R.t_b \mid x_L.t_a) &= \int\int \frac{\mathcal{D}x\mathcal{D}p}{2\pi\hbar}\; e^{\frac{i}{\hbar}\int_{t_a}^{t_b} dt(p\dot{x}-H(x,p))} \\
&= \left(\prod_{n=1}^{N-1}\int_{-\infty}^{+\infty} dx_n\right)\prod_{n=1}^{N}\left(\int_{-\infty}^{+\infty}\frac{dp_n}{2\pi\hbar}\; e^{\frac{i}{\hbar}\epsilon\left(p_n\dot{x}_n-\frac{p_n^2}{2m}\right)} e^{-\frac{i}{\hbar}\epsilon V(x_{n-1})}\right) \\
&= \left(\prod_{n=1}^{N-1}\int_{-\infty}^{+\infty} dx_n\right)\prod_{n=1}^{N}\left(\int_{-\infty}^{+\infty}\frac{dp_n}{2\pi\hbar}\; e^{-\frac{i}{2m\hbar}\epsilon\left(p_n^2-2mp_n\dot{x}_n+\underbrace{(m\dot{x}_n)^2-(m\dot{x}_n)^2}_{=0}\right)} e^{-\frac{i}{\hbar}\epsilon V(x_{n-1})}\right) \\
&= \left(\prod_{n=1}^{N-1}\int_{-\infty}^{+\infty} dx_n\, e^{-\frac{i}{\hbar}\epsilon V(x_{n-1})}\, e^{\frac{i}{2m\hbar}\epsilon(m\dot{x}_n)^2}\right)\prod_{n=1}^{N}\left(\int_{-\infty}^{+\infty}\frac{dp_n}{2\pi\hbar}\; e^{-\frac{i}{2m\hbar}\epsilon(p_n-m\dot{x}_n)^2}\right) = \dots
\end{aligned} \tag{23}$$

Two steps of using Gaussian integrals simplify this to

$$
\begin{aligned}
\ldots &= \left(\prod_{n=1}^{N-1} \int_{-\infty}^{+\infty} dx_n \, e^{\frac{i}{\hbar}\epsilon\left(\frac{m}{2}\dot{x}_n^2 - V(x_{n-1})\right)}\right) \prod_{n=1}^{N} \frac{1}{2\pi\hbar} \sqrt{\frac{\pi}{\frac{i}{2m\hbar}\epsilon}} \\
&= \prod_{n=1}^{N-1} \int_{-\infty}^{+\infty} dx_n \sqrt{\frac{m}{2\pi i\hbar\epsilon}} \; e^{\frac{i}{\hbar}\epsilon\left(\frac{m}{2}\dot{x}_n^2 - V(x_{n-1})\right)} \\
&= \int \mathcal{D}x \; e^{\frac{i}{\hbar}\int_{t_a}^{t_b} dt\left(\frac{m}{2}\dot{x}^2 - V(x)\right)} .
\end{aligned}
\tag{24}
$$

In the last step, we used the refined path integral notation

$$
\prod_{n=1}^{N-1} \int_{-\infty}^{+\infty} dx_n \sqrt{\frac{m}{2\pi i\hbar\epsilon}} =: \int \mathcal{D}x \;\; \text{for } N \to \infty. \tag{25}
$$

Note that while the path integral operation $\int \mathcal{D}x$ is still dimensionless, it has an implicit dependence on the mass m that stems from the mass dependency of the momentum which we just got rid of.

This form of the path integral doesn't include the integral over all possible paths in the momentum space any more and therefore is way easier to handle. It also doesn't incorporate boundary conditions for the momentum, but those can be processed physically correctly by applying them on $\dot{x} \hat{=} \frac{p}{m}$.

Now the problem is that we do not really have an overview on how the phase $\frac{i}{\hbar}\int_{t_a}^{t_b} dt\,(p\dot{x} - H(x,p))$ behaves for the totality of the vast collection of paths in position and momentum space. Additionally, we cannot ensure the path integral's meaningful convergence. An idea to solve this issue is to rewrite the integrations in such a way that the contributions of as many alternative paths as possible cancel out and only a few dominating ones remain, that might have a somewhat controlled phase.

3 The Saddle Point Method

The saddle point method is a tool to approximate integrals of the form

$$I(k) = \int_{x_1}^{x_2} dx f(x) e^{k^2 g(x)} \tag{26}$$

for large k. The premises are that f and g are analytic functions $\mathbb{R} \longrightarrow \mathbb{R}$ and that we know the global maximum x_0 of g with $x_1 < x_0 < x_2$ and $f(x_0) \neq 0$. Then we use Taylor expansion of g around x_0 to get the value in dependence of k:
Let $r = k(x - x_0)$, $dx = \frac{dx}{dr} dr = \frac{dr}{k}$, $r_1 = k(x_1 - x_0)$, $r_2 = k(x_2 - x_0)$. Hence

$$\begin{aligned} k^2 g(x) = k^2 g(x_0) + k^2(x - x_0) \underbrace{g'(x_0)}_{=0} + k^2 (x - x_0)^2 \frac{g''(x_0)}{2} \\ + k^2 (x - x_0)^3 \frac{g'''(x_0)}{6} + k^2 (x - x_0)^4 \frac{g''''(x_0)}{24} + \dots \end{aligned} \tag{27}$$

$$= k^2 g(x_0) + r^2 \frac{g''(x_0)}{2} + k^{-1} r^3 \frac{g'''(x_0)}{6} + k^{-2} r^4 \frac{g''''(x_0)}{24} + \dots \tag{28}$$

and thus

$$e^{k^2 g(x)} = e^{k^2 g(x_0) + r^2 \frac{g''(x_0)}{2}} e^{k^{-1} r^3 \frac{g'''(x_0)}{6} + r^4 k^{-2} \frac{g''''(x_0)}{24} + \dots} \tag{29}$$

$$= e^{k^2 g(x_0) + r^2 \frac{g''(x_0)}{2}} \left(1 + k^{-1} (r^3 \frac{g'''(x_0)}{6}) + k^{-2} (r^6 \frac{g'''(x_0)^2}{72} + r^4 \frac{g''''(x_0)}{24}) + \dots \right). \tag{30}$$

Similarly, the expansion of f gives

$$f(x) = f(x_0) + (x - x_0)f'(x_0) + (x - x_0)^2\frac{f''(x_0)}{2} + (x - x_0)^3\frac{f'''(x_0)}{6} + \dots \tag{31}$$

$$= f(x_0) + k^{-1}rf'(x_0) + k^{-2}r^2\frac{f''(x_0)}{2} + k^{-3}r^3\frac{f'''(x_0)}{6} \tag{32}$$

$$= f(x_0)\left(1 + k^{-1}r\frac{f'(x_0)}{f(x_0)} + k^{-2}r^2\frac{f''(x_0)}{2f(x_0)} + k^{-3}r\frac{f'''(x_0)}{6f(x_0)} + \dots\right), \tag{33}$$

and the integral becomes

$$I(k) = \int_{x_1}^{x_2} dxf(x)e^{k^2 g(x)}$$

$$= \int_{x_1}^{x_2} dxf(x_0)\left(1 + k^{-1}r\frac{f'(x_0)}{f(x_0)} + k^{-2}r^2\frac{f''(x_0)}{2f(x_0)} + \dots\right)$$

$$\cdot\, e^{k^2 g(x_0) + r^2\frac{g''(x_0)}{2}}\left(1 + k^{-1}(r^3\frac{g'''(x_0)}{6}) + k^{-2}\cdots + \dots\right)$$

$$= \frac{f(x_0)e^{k^2 g(x_0)}}{k}\int_{r_1}^{r_2} dre^{r^2\frac{g''(x_0)}{2}}\left(1 + \sum_{n=1}^{\infty} k^{-n}P_n(r)\right), \tag{34}$$

where P_n are fixed polynomials that can be calculated (with dependence on the derivatives of f and g at x_0), which are odd for odd n and even for even n. The limit for very large k means for the integration limits that $r_1 = k(x_1 - x_0)$ tends towards $-\infty$ and $r_2 = k(x_1 - x_0)$ towards $+\infty$. As the term $e^{r^2\frac{g''(x_0)}{2}}$ gets very small very fast for large r (since $g''(x_0)$ is negative because we have a maximum), it doesn't make a big difference if we integrate from $-\infty$ to $+\infty$ instead of from r_1 to r_2. This makes it a Gaussian integral where the summands with odd n result in integral values of zero.

It evaluates to

$$I(A) = \frac{f(x_0) e^{k^2 g(x_0)}}{k} \int\limits_{-\infty}^{+\infty} dr e^{r^2 \frac{g''(x_0)}{2}} \left(1 + \sum_{n=1}^{\infty} k^{-n} P_n(r)\right) \tag{35}$$

$$= f(x_0) e^{k^2 g(x_0)} \sqrt{\frac{2\pi}{-k^2 g''(x_0)}} \left(1 + \sum_{n=1}^{\infty} k^{-n} C_{2n}\right) \tag{36}$$

with some constants C_n that can be calculated from the given functions. In general, the series $\sum_{n=1}^{\infty} k^{-2n} C_{2n}$ has zero radius of convergence, but we still have

$$\sum_{n=1}^{\infty} k^{-2n} C_{2n} = \sum_{n=1}^{k-1} k^{-2n} C_{2n} + \mathcal{O}(k^{-2k}) \tag{37}$$

in the strict mathematical sense of $\mathcal{O}$. Thus we can write

$$I(A) = f(x_0) e^{k^2 g(x_0)} \sqrt{\frac{2\pi}{-k^2 g''(x_0)}} \left(1 + \frac{C_2}{k^2} + \mathcal{O}(k^{-4})\right). \tag{38}$$

With this, we have found an approximation for the integral which can be calculated quickly from the values of the first few derivatives of f and g at the global maximum x_0 of g and that becomes accurate for large k.

4 The Method of Wick Rotation

We present method that is commonly used to calculate the path integral

$$(x_R.t_b|x_L.t_a) = \int \mathcal{D}x\ e^{\frac{i}{\hbar}\int\limits_{t_a}^{t_b} dt\left(\frac{m}{2}\dot{x}^2 - V(x)\right)}. \tag{39}$$

It essentially consists of rotating the direction of time integration $\int\limits_{t_a}^{t_b} dt$ from the real to the imaginary axis. Descriptions of this method are given in most books on path integrals, for example [Kleinert, 1995] and [Altland and Simons, 2010], or in the article [Tanizaki and Koike, 2014].

First, the integration variable $\tau := i(t - \frac{t_b+t_a}{2})$ is introduced; then

$$dt = \frac{dt}{d\tau}d\tau = -id\tau, \tag{40}$$

while the integration limits become $i\frac{L}{2}$ and $-i\frac{L}{2}$ with $L := t_b - t_a$, and $\dot{x}$ can be expressed as

$$\dot{x} = \frac{dx}{dt} = \frac{dx}{-id\tau} = i\frac{dx}{d\tau} =: ix'. \tag{41}$$

Thus the time integral can be rewritten

$$\frac{i}{\hbar}\int\limits_{t_a}^{t_b} dt\left(\frac{m\dot{x}^2}{2} - V(x)\right) = \frac{i}{\hbar}\int\limits_{-i\frac{L}{2}}^{i\frac{L}{2}} -id\tau\left(\frac{-mx'^2}{2} - V(x)\right) = \frac{-1}{\hbar}\int\limits_{-i\frac{L}{2}}^{i\frac{L}{2}} d\tau\left(\frac{mx'^2}{2} + V(x)\right). \tag{42}$$

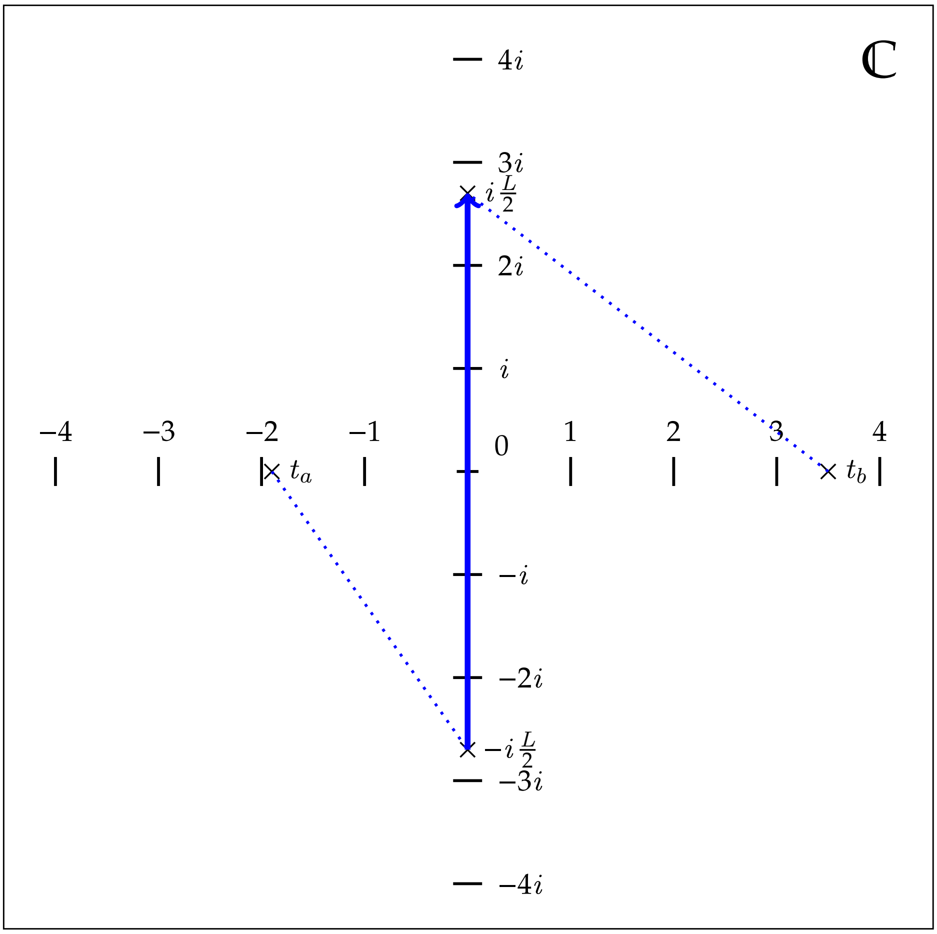

Figure 1: The imaginary integration path

As expressed by the imaginary integration limits, the integral is taken along the imaginary axis now, as pictured in figure 1. Note that the integral $\frac{-1}{\hbar}\int_{-i\frac{L}{2}}^{i\frac{L}{2}} d\tau(\frac{mx'^2}{2} + V(x))$ still evaluates to the same number, due to the imaginary integration path, and hence still assumes imaginary values. Here is where the crucial trick happens: calculating the transition probability $(x_R.{-i\frac{L}{2}}|x_L.i\frac{L}{2})$ between states in imaginary time instead of the number $(x_R.t_b|x_L.t_a)$ that we are finally interested in.

Ultimately, it is possible to calculate the value of $(x_R.{-i\frac{L}{2}}|x_L.i\frac{L}{2})$ as a function of it_a and it_b. It will eventually still be smooth and can be analytically continued to a holomorphic function, allowing its evaluation at the real time values which we are actually interested in.

The Wick rotation is done by simply replacing the times t_a with $i\frac{L}{2}$ and t_b with $i\frac{L}{2}$ in the previous considerations, which leads to the expression

$$(x_R.i\frac{L}{2}|x_L.-i\frac{L}{2}) = \int\int \mathcal{D}x \, \frac{\mathcal{D}p}{2\pi\hbar} \, e^{\frac{-1}{\hbar}\int_{-\frac{L}{2}}^{\frac{L}{2}} d\tau(\frac{mx'^2}{2}+V(x))}. \tag{43}$$

Now the exponent assumes real values and the path integral as a whole resembles the real integral in equation 26. This allows us to use the saddle point method: The transition probability can be determined by only regarding the paths where the action

$$S = \int_{-\frac{L}{2}}^{\frac{L}{2}} d\tau \left(\frac{mx'^2}{2} + V(x)\right) \tag{44}$$

is minimal under small variations. If we compare this expression with the original action, we see that what happened is that the minus sign in front of the potential switched to a plus sign. Hence the action extremization problem can be interpreted as that of the original potential flipped over the x-axis. The variations of paths correspond to the derivatives in the treatment of non-functional integrals. We use the name $x_c(\tau)$ for this path that minimizes the problem's action: $0 = \int_{-\frac{L}{2}}^{\frac{L}{2}} d\tau \left(\frac{m\delta x_c'^2}{2} + V(\delta x_c)\right)$. Finding this path is the classical problem of finding the equation of motion for the given Lagrange function $L = \frac{mx'^2}{2} + V(x)$. The solution is given by the Euler-Lagrange equation

$$-mx'' + \frac{dV}{dx}(x) = 0. \tag{45}$$

Multiplication of this equation with x' yields

$$-mx''x' + \frac{dV}{dx}(x)x' = 0 \tag{46}$$

which when integrated over time results in

$$0 = \int_{-\frac{L}{2}}^{\tau} d\tau'(-mx''x' + \frac{dV}{dx}(x)x') = \Big[-\frac{mx'^2}{2} + V(x)\Big]_{-\frac{L}{2}}^{\tau} \tag{47}$$

$$= -\frac{mx'(\tau)^2}{2} + V(x(\tau)) + \frac{mx'(-\frac{L}{2})^2}{2} - V(x(-\frac{L}{2})). \tag{48}$$

If we look at the infinite time limit, i.e. $t_b - t_a = L \to \infty$, and if we assume one single tunneling process while the particle is at rest at the point $-a$ (where the potential energy is set to 0) for large negative times, then the lower integration boundary terms are 0 and the minimising path x_c satisfies

$$V(x_c) = \frac{mx_c'^2}{2}. \tag{49}$$

After we have found this minimizing path, we insert equation 49 into equation 44 and get the saddle point action

$$S_c = \int_{-\frac{L}{2}}^{\frac{L}{2}} d\tau(mx_c'^2). \tag{50}$$

5 Wick Rotation for a Particle in a Double Well Potential

We want to calculate the transition probability for the Hamiltonian

$$H = \frac{P^2}{2m} + \kappa(X + a)^2(X - a)^2 \tag{51}$$

and $x_L = -a$, $x_R = a$ in a time span $L = t_b - t_a$ with the momentum and hence the total energy being zero at the beginning, as done in for example in [Kleinert, 1995] and [Cherman and Ünsal, 2014].

The Hamiltonian given by equation 51 describes a particle in a double well potential as shown in figure 2.

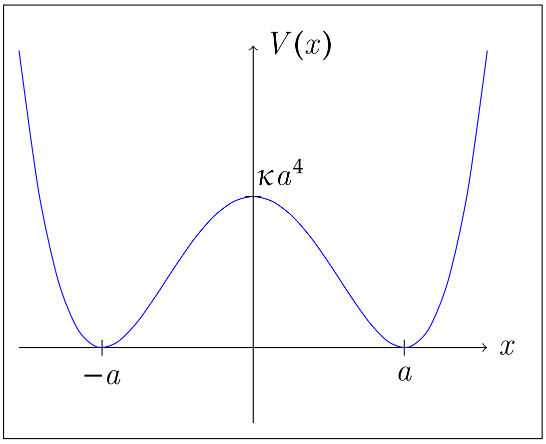

Figure 2: The Potential $V(x) = \kappa(x+a)^2(x-a)^2$

The path integral formalism states that the transition amplitude is

$$(a.t_b|-a.t_a) = \int \mathcal{D}x \; e^{\frac{i}{\hbar}S[x]} \tag{52}$$

where for the regarded double well potential the classical action is

$$S[x] = \int_{t_a}^{t_b} dt \left(m\dot{x}^2 - \left(\frac{m\dot{x}^2}{2} + \kappa(x+a)^2(x-a)^2 \right) \right) = \int_{t_a}^{t_b} dt \left(\frac{m\dot{x}^2}{2} - \kappa(x^2-a^2)^2 \right). \tag{53}$$

We are interested in the limit probability $(a.\infty|-a.-\infty)$ of the particle tunnelling from the bottom of the left to the bottom of the right valley given infinite time.

To do this, we apply the Wick rotation as introduced in section 4, i.e. we rotate the paths $x(t)$ to imaginary time by changing the time integration limits:

$$(a.i\infty|-a.-i\infty) = \int \mathcal{D}x \; e^{\frac{i}{\hbar}\int\limits_{-i\infty}^{i\infty} dt\left(\frac{m(\frac{\partial x}{\partial t})^2}{2} - \kappa(x^2-a^2)^2\right)}. \tag{54}$$

Writing $\tau = it$ helps us simplify the exponent

$$\begin{aligned} \frac{i}{\hbar}\int\limits_{-i\infty}^{i\infty} dt\left(\frac{m(\frac{\partial x}{\partial t})^2}{2} - \kappa(x^2-a^2)^2\right) &= \frac{i}{\hbar}\int\limits_{-i\infty}^{i\infty} -i\; idt\left(\frac{-m(\frac{\partial x}{\partial it})^2}{2} - \kappa(x^2-a^2)^2\right) \\ &= \frac{1}{\hbar}\int\limits_{-\infty}^{\infty} d\tau\left(\frac{-m(\frac{\partial x}{\partial \tau})^2}{2} - \kappa(x^2-a^2)^2\right) \\ &= \frac{-1}{\hbar} S_E[x], \end{aligned} \tag{55}$$

where

$$S_E[x] = \int\limits_{-\infty}^{\infty} d\tau\left(\frac{m}{2}(\frac{\partial x}{\partial \tau})^2 + \kappa(x^2-a^2)^2\right). \tag{56}$$

Ultimately, the path integral has the form

$$(a.i\infty|-a.-i\infty) = \int \mathcal{D}x \; e^{\frac{1}{\hbar}S_E[x]}. \tag{57}$$

Assuming that $\frac{1}{\hbar}$ is very big in comparison with typical absolute values of the action, the idea is to use the saddle point method, looking only at those paths x that minimize $S_E[x]$. Finding such a trajectory which is minimizing the action is done by solving the

Euler-Lagrange equation

$$0 = \frac{\partial L}{\partial x} - \frac{d}{d\tau}\frac{\partial L}{\partial\left(\frac{\partial x}{\partial \tau}\right)}, \tag{58}$$

where $L(x, \frac{\partial x}{\partial \tau}, \tau)$ is the integrand in the action integral, in our case $L = \frac{m}{2}(\frac{\partial x}{\partial \tau})^2 + \kappa(x^2 - a^2)^2$. Thus, we need to look for trajectories $x(\tau)$ that fulfill

$$0 = 4\kappa x(x^2 - a^2) - 2\frac{m}{2}\frac{\partial^2 x}{\partial \tau^2}. \tag{59}$$

We set

$$\lambda := \sqrt{\frac{2\kappa}{m}}. \tag{60}$$

The second order differential equation

$$\frac{\partial^2 x}{\partial \tau^2} = 2\lambda^2 x(x^2 - a^2), \tag{61}$$

with the boundary condition $\frac{\partial x}{\partial \tau}(\tau = -\infty) = 0$ that the particle is at rest at the beginning, is solved by

$$x(\tau) = a \tanh(\lambda a(\tau - \tau_0)), \tag{62}$$

as we show in the following calculation:

$$\begin{aligned} \frac{\partial^2 (a \tanh \lambda a\tau)}{\partial \tau^2} &= \lambda^2 a^3 \frac{\partial^2 \frac{\sinh \lambda a\tau}{\cosh \lambda a\tau}}{(\partial(\lambda a\tau))^2} \\ &= \lambda^2 a^3 \frac{\partial}{\partial(\lambda a\tau)} \frac{\cosh^2 \lambda a\tau - \sinh^2 \lambda a\tau}{\cosh^2 \lambda a\tau} \\ &= \lambda^2 a^3 \frac{\partial}{\partial(\lambda a\tau)}(1 - \tanh^2 \lambda a\tau) \\ &= \lambda^2 a^3 2 \tanh \lambda a\tau \,(\tanh^2 \lambda a\tau - 1) \\ &= 2\lambda^2 (a \tanh \lambda a\tau)\,((a \tanh \lambda a\tau)^2 - a^2). \end{aligned} \tag{63}$$

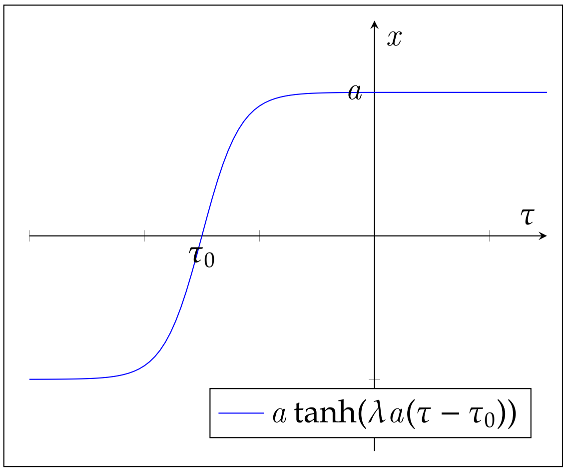

Figure 3: A solution for infinite imaginary time

The parameter τ_0 surely doesn't alter the property of being a solution for differential equation 61, but it gives us a degree of freedom which makes sense, physically as we calculate the total probability of tunneling at any arbitrary time, and mathematically as we deal with a 2nd order linear differential equation with 1 boundary condition. Note that $x(\tau) = -a\tanh(\lambda a(\tau - \tau_0))$ would solve the differential equation 61 as well, but since it isn't in accord with the problem's boundary condition of the particle starting at $-a$ and ending up at $+a$, we do not need to regard this solution.

A plot of this solution is shown in figure 3. An interpretation is that the particle stays close to its starting point for a long time, then switches to the other well very rapidly and stays there forever without going back and forth.

Now we calculate the (rotated) action of this solution by inserting it into equation 56:

$$
\begin{aligned}
S_E[a\tanh\lambda a\tau] &= \int_{-\infty}^{\infty} d\tau \left(\frac{m}{2}(\frac{a\tanh\lambda a\tau}{\partial\tau})^2 + \kappa((a\tanh\lambda a\tau)^2 - a^2)^2\right) \\
&= \int_{-\infty}^{\infty} d\tau \left(\frac{m}{2}(\lambda a^2(1-\tanh^2\lambda a\tau))^2 + \kappa(a^2(\tanh^2\lambda a\tau - 1))^2\right) \\
&= 2\kappa a^4 \int_{-\infty}^{\infty} d\tau(1-\tanh^2\lambda a\tau)^2 \\
&= 2\kappa a^4 \int_{-\infty}^{\infty} d\tau(1-\tanh^2\lambda a\tau)\frac{\partial(\tanh\lambda a\tau)}{\partial\lambda a\tau} \\
&= 2\frac{\kappa}{\lambda}a^3 \int_{-\infty}^{\infty} (1-\tanh^2\lambda a\tau)\ d(\tanh\lambda a\tau) \\
&= \ \sqrt{2m\kappa}\ a^3\Big[\tanh\lambda a\tau - \frac{1}{3}\tanh^3\lambda a\tau\Big]_{-\infty}^{+\infty} \\
&= \ \sqrt{2m\kappa}a^3(1-\frac{1}{3}-(1-\frac{1}{3})) \\
&= \frac{8}{3}\sqrt{2m\kappa}a^3
\end{aligned}
\tag{64}
$$

6 Trying the Same Approach While Staying in Real Time

If we try to do the same calculation for the non-rotated action $S[x]$ in 53, we end up with the Euler-Lagrange equation

$$
-\frac{\partial^2 x}{\partial t^2} = 2\lambda^2 x(x^2 - a^2). \tag{65}
$$

It is the same as for the rotated, Euclidean action except for the minus sign in front of the second derivative. The solution that is analogous to the hyperbolic tangent function from above is $x(t) = \pm ia \tan \lambda a(t - t_0)$. This can be seen easily as

$$\begin{aligned} \tan \lambda at &= \frac{\sin \lambda at}{\cos \lambda at} = \frac{e^{i\lambda at} - e^{-i\lambda at}}{i(e^{i\lambda at} + e^{-i\lambda at})} \\ &= \frac{\sinh i\lambda at}{i \cosh i\lambda at} = -i \tanh i\lambda at \end{aligned} \tag{66}$$

and thus

$$\begin{aligned} -\frac{\partial^2(ia \tan \lambda at)}{\partial t^2} &= -\frac{\partial^2(a \tanh \lambda ait)}{-\partial(it)^2} \\ &\overset{63}{=} 2\lambda^2(a \tanh \lambda ait)\,((a \tanh \lambda ait)^2 - a^2) \\ &= 2\lambda^2(ia \tan \lambda at)\,((ia \tan \lambda at)^2 - a^2). \end{aligned} \tag{67}$$

The issue with this $\pm ia \tan a(t - t_0)$ solution is that it describes a path on the imaginary axis that even has singularities. Hence, there is no apparent way to interpret it as connecting the real points $-a$ and $+a$. As there are no other physical solutions for equation 65, we have to conclude that the direct approach of using the saddle-point/Euler-Lagrange method on the original, not rotated problem doesn't produce a solution path.

7 Between Imaginary and Real Time

In order to receive a meaningful path that is minimizing the action, we rotated the time axis from purely real to purely imaginary values. This corresponds to a rotation by an angle of $\phi = \frac{\pi}{2}$ in the complex plane, or a multiplication with the phase factor $e^{\frac{\pi}{2}i}$. Now that we know that we get a solution for $\phi = \frac{\pi}{2}$, which is unfortunately very distinct from the not rotated case $\phi = 0$ that represents our actual problem, the idea is to inspect what lies in between the two angles. By this we mean to allow any value for ϕ and to see what we get for $(a.e^{\phi i}\infty|-a.-e^{\phi i}\infty)$. This section's deductions are based on [Cherman and Ünsal, 2014]. Just as in equation 54, the expression for this sloped time axis integral is

$$(a.e^{\phi i}\infty|-a.-e^{\phi i}\infty) = \int \mathcal{D}x\ e^{\frac{i}{\hbar}\int_{e^{\phi i}\infty}^{-e^{\phi i}\infty} dt\left(\frac{m(\frac{\partial x}{\partial t})^2}{2}-\kappa(x^2-a^2)^2\right)}. \tag{68}$$

We rewrite the action (this time setting $\tau = e^{\phi i}$):

$$\begin{aligned} S_\phi[x] &= \int_{-e^{\phi i}\infty}^{e^{\phi i}\infty} dt\left(\frac{m(\frac{\partial x}{\partial t})^2}{2} - \kappa(x^2-a^2)^2\right) \\ &= \int_{-e^{\phi i}\infty}^{e^{\phi i}\infty} e^{-\phi i}e^{\phi i}dt\left(\frac{me^{2\phi i}\left(\frac{\partial x}{\partial(e^{\phi i}t)}\right)^2}{2} - \kappa(x^2-a^2)^2\right) \\ &= e^{-\phi i}\int_{-\infty}^{\infty} d\tau\left(\frac{me^{2\phi i}\left(\frac{\partial x}{\partial \tau}\right)^2}{2} - \kappa(x^2-a^2)^2\right). \end{aligned} \tag{69}$$

This produces the Euler-Lagrange equation

$$0 = -4\kappa x(x^2-a^2) - 2e^{2\phi i}\frac{m}{2}\frac{\partial^2 x}{\partial \tau^2}, \tag{70}$$

or

$$-e^{2\phi i}\frac{\partial^2 x}{\partial \tau^2} = 2\lambda x(x^2-a^2). \tag{71}$$

It is solved by $x(\tau) = \pm a \tanh(e^{-(\phi-\frac{\pi}{2})i}\lambda a(\tau - \tau_0))$, as we see similar as before that

$$\begin{aligned} -e^{2\phi i}\frac{\partial^2(a \tanh e^{-(\phi-\frac{\pi}{2})i}\lambda a\tau)}{\partial\tau^2} &= i\frac{\partial^2(ia \tanh e^{-\phi i} i\lambda a\tau)}{\partial(e^{-\phi i}\tau)^2} \\ &\overset{63}{=} 2\lambda i(ia \tanh e^{-\phi i} i\lambda a\tau)\,((ia \tanh e^{-\phi i} i\lambda a\tau)^2 - (ia)^2) \\ &= 2\lambda(a \tanh e^{-(\phi-\frac{\pi}{2})i}\lambda a\tau)\,((a \tanh e^{-(\phi-\frac{\pi}{2})i}\lambda a\tau)^2 - a^2). \end{aligned} \tag{72}$$

Above, we have seen that this solution doesn't connect $-a$ with a in the infinite time limit if we set $\phi = 0$, but does is perfectly for $\phi = \frac{\pi}{2}$. What happens for other values of ϕ?

We use Euler's formula to expand

$$e^{-(\phi-\frac{\pi}{2})i} = \cos(\phi - \frac{\pi}{2}) - i\sin(\phi - \frac{\pi}{2}) =: c - is \tag{73}$$

and have

$$\begin{aligned} \tanh(e^{-(\phi-\frac{\pi}{2})i}\lambda a\tau) &= \frac{e^{(c-is)\lambda a\tau} - e^{-(c-is)\lambda a\tau}}{e^{(c-is)\lambda a\tau} + e^{-(c-is)\lambda a\tau}} \\ &= \frac{e^{c\lambda a\tau}e^{-is\lambda a\tau} - e^{-c\lambda a\tau}e^{is\lambda a\tau}}{e^{c\lambda a\tau}e^{-is\lambda a\tau} + e^{-c\lambda a\tau}e^{is\lambda a\tau}}. \end{aligned} \tag{74}$$

The limit for $\tau \longrightarrow \infty$ depends on the sign of c:

For $c > 0$ $\frac{e^{c\lambda a\tau}e^{-is\lambda a\tau} - e^{-c\lambda a\tau}e^{is\lambda a\tau}}{e^{c\lambda a\tau}e^{-is\lambda a\tau} + e^{-c\lambda a\tau}e^{is\lambda a\tau}} \xrightarrow{\tau\to\infty} \frac{e^{c\lambda a\tau}e^{-is\lambda a\tau}}{e^{c\lambda a\tau}e^{-is\lambda a\tau}} = 1$

For $c < 0$ $\frac{e^{c\lambda a\tau}e^{-is\lambda a\tau} - e^{-c\lambda a\tau}e^{is\lambda a\tau}}{e^{c\lambda a\tau}e^{-is\lambda a\tau} + e^{-c\lambda a\tau}e^{is\lambda a\tau}} \xrightarrow{\tau\to\infty} \frac{-e^{-c\lambda a\tau}e^{is\lambda a\tau}}{e^{-c\lambda a\tau}e^{is\lambda a\tau}} = -1$

For $c = 0$ $\frac{e^{c\lambda a\tau}e^{-is\lambda a\tau} - e^{-c\lambda a\tau}e^{is\lambda a\tau}}{e^{c\lambda a\tau}e^{-is\lambda a\tau} + e^{-c\lambda a\tau}e^{is\lambda a\tau}} = \frac{e^{-is\lambda a\tau} - e^{is\lambda a\tau}}{e^{-is\lambda a\tau} + e^{is\lambda a\tau}} = -si\tan\lambda a\tau$, as of course $c = 0$ means $s = 1$ or $s = -1$.

After doing analogous considerations for $\tau \to -\infty$, as a result we get the following table:

ϕ (mod 2π)	$a\tanh(e^{-(\phi-\frac{\pi}{2})i}\lambda a\tau)$ $\tau \to -\infty$	$a\tanh(e^{-(\phi-\frac{\pi}{2})i}\lambda a\tau)$ $\tau \to +\infty$	$-a\tanh(e^{-(\phi-\frac{\pi}{2})i}\lambda a\tau)$ $\tau \to -\infty$	$-a\tanh(e^{-(\phi-\frac{\pi}{2})i}\lambda a\tau)$ $\tau \to +\infty$
$0 < \phi < \pi$	$-a$	$+a$	$+a$	$-a$
$\pi < \phi < 2\pi$	$+a$	$-a$	$-a$	$+a$
$\phi = 0$	$ia\tan\lambda a\tau$	$ia\tan\lambda a\tau$	$-ia\tan\lambda a\tau$	$-ia\tan\lambda a\tau$
$\phi = \pi$	$-ia\tan\lambda a\tau$	$-ia\tan\lambda a\tau$	$ia\tan\lambda a\tau$	$ia\tan\lambda a\tau$

Thus, the solutions that connect $-a$ with $+a$ are $x(\tau) = a\tanh(e^{-(\phi-\frac{\pi}{2})i}\lambda a(\tau-\tau_0))$ in the case $0 < \phi < \pi$ and $x(\tau) = -a\tanh(e^{-(\phi-\frac{\pi}{2})i}\lambda a(\tau-\tau_0))$ in the case $\pi < \phi < 2\pi$, while for the original problem $\phi = 0$, there is no solution of this type.

To connect this path with a transition probability, we need to calculate its action. It is

$$
\begin{aligned}
S_\phi[a\tanh e^{-(\phi-\frac{\pi}{2})i}\lambda a\tau] &= e^{-\phi i}\int_{-\infty}^{\infty} d\tau\left(\frac{me^{2\phi i}\left(\frac{\partial x}{\partial\tau}\right)^2}{2} - \kappa(x^2-a^2)^2\right)\\
&= e^{-\phi i}\int_{-\infty}^{\infty} d\tau\left(\frac{me^{2\phi i}}{2}\left(\frac{\partial(a\tanh e^{-(\phi-\frac{\pi}{2})i}\lambda a\tau)}{\partial\tau}\right)^2 - \kappa((a\tanh e^{-(\phi-\frac{\pi}{2})i}\lambda a\tau)^2-a^2)^2\right)\\
&= e^{-\phi i}\int_{-\infty}^{\infty} d\tau\left(\frac{me^{2\phi i}}{2}(e^{-(\phi-\frac{\pi}{2})i}\lambda a^2(1-\tanh^2 e^{-(\phi-\frac{\pi}{2})i}\lambda a\tau))^2 - \kappa(a^2(\tanh^2 e^{-(\phi-\frac{\pi}{2})i}\lambda a\tau - 1))^2\right)\\
&= e^{-\phi i}\int_{-\infty}^{\infty} d\tau\left(\frac{me^{2\phi i}e^{-2\phi i}e^{\pi i}}{2}(\lambda a^2(1-\tanh^2 e^{-(\phi-\frac{\pi}{2})i}\lambda a\tau))^2 - \kappa(a^2(\tanh^2 e^{-(\phi-\frac{\pi}{2})i}\lambda a\tau - 1))^2\right)
\end{aligned}
$$

$$
\begin{aligned}
&= -2e^{-\phi i}\kappa a^4 \int\limits_{-\infty}^{\infty} d\tau (1-\tanh^2 e^{-(\phi-\frac{\pi}{2})i}\lambda a\tau)^2 \\
&= -2e^{-\phi i}\kappa a^4 \int\limits_{-\infty}^{\infty} d\tau (1-\tanh^2 e^{-(\phi-\frac{\pi}{2})i}\lambda a\tau) \frac{\partial(\tanh e^{-(\phi-\frac{\pi}{2})i}\lambda a\tau)}{\partial e^{-(\phi-\frac{\pi}{2})i}\lambda a\tau} \\
&= -2e^{-\phi i}\frac{\kappa}{e^{-(\phi-\frac{\pi}{2})i}\lambda} a^3 \int\limits_{-\infty}^{\infty} (1-\tanh^2 e^{-(\phi-\frac{\pi}{2})i}\lambda a\tau)\; d(\tanh e^{-(\phi-\frac{\pi}{2})i}\lambda a\tau) \\
&= \sqrt{2m\kappa}\; a^3 \Big[\tanh e^{-(\phi-\frac{\pi}{2})i}\lambda a\tau - \frac{1}{3}\tanh^3 e^{-(\phi-\frac{\pi}{2})i}\lambda a\tau\Big]_{-\infty}^{+\infty} \\
&= \sqrt{2m\kappa} a^3 (1-\frac{1}{3}-(1-\frac{1}{3})) \quad (\text{for } 0<\phi<\pi) \\
&= \frac{8}{3}\sqrt{2m\kappa} a^3
\end{aligned} \tag{75}
$$

In the second to last step, we worked in the area $0 < \phi < \pi$ where $a \tanh e^{-(\phi-\frac{\pi}{2})i}\lambda a\tau$ is the connecting, action minimizing path. For $\pi < \phi < 2\pi$, we get a minus sign here that cancels out with the one we get for taking the $-a \tanh e^{-(\phi-\frac{\pi}{2})i}\lambda a\tau$ solution, and the action is the same.

The interesting point about this is that the action does not depend on the angle ϕ at all. This means that $S_\phi[a \tanh e^{-(\phi-\frac{\pi}{2})i}\lambda a\tau]$, if seen as a function of ϕ which is defined for $\phi \neq n\pi$, is constant and thus can easily be analytically continued in $\phi = 0$ with the same value. Hence, for calculating the transition probability, the rotation angle is not important and we can readily calculate it with a rotated path. Thus, we only need a reason why a rotated path is physical; for this, any ever so small rotation would be sufficient.

8 The Divergence of $a\tanh(e^{-(\phi-\frac{\pi}{2})i}\lambda a(\tau+\tau_0))$ for $\phi \to 0$

We want to understand what happens when ϕ approaches and becomes zero and where this discontinuous behavior of the end points jumping from the real to the imaginary axis arises from. So let us look at how the graphs of $a\tanh(e^{-(\phi-\frac{\pi}{2})i}\lambda a(\tau+\tau_0))$ with $a = 1$, $\lambda = 1$ and $\tau_0 = 0$ are shaped for some values of ϕ.

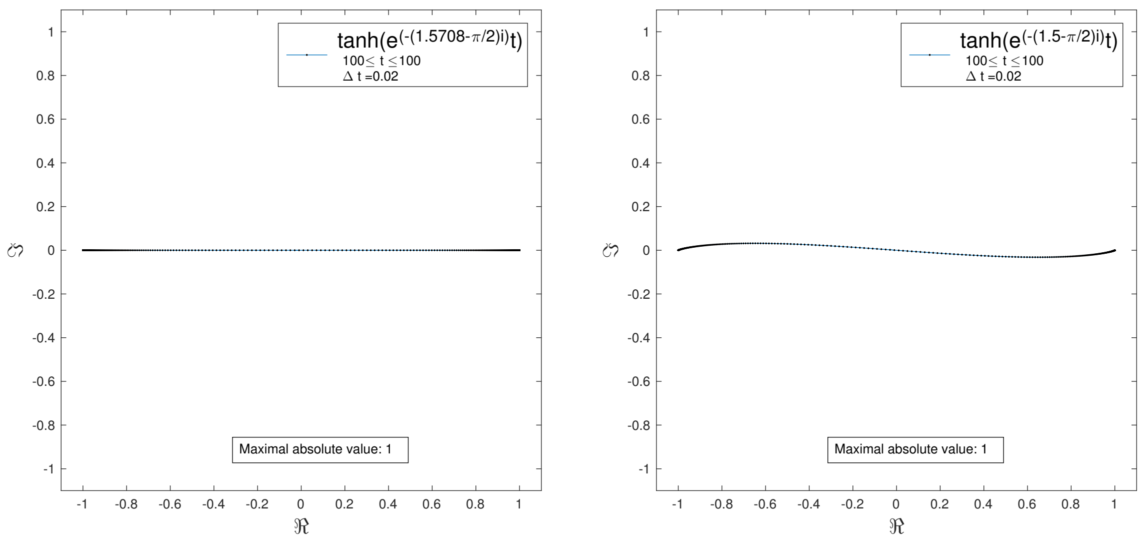

Figure 4: Trajectories for $\phi = \frac{\pi}{2}$ and $\phi = 1.5$

In figure 4 we have drawn the path of motion in the complex plane for $\phi = \frac{\pi}{2}$ and for $\phi = 1.5$ with MATLAB R2013a. The $\frac{\pi}{2}$-case, as discussed in section 5, just produces a line from -1 to $+1$ that lies straight on the real axis. For the a little smaller angle of $\phi = 1.5$ we see a little bend through regions with non-vanishing imaginary parts already.

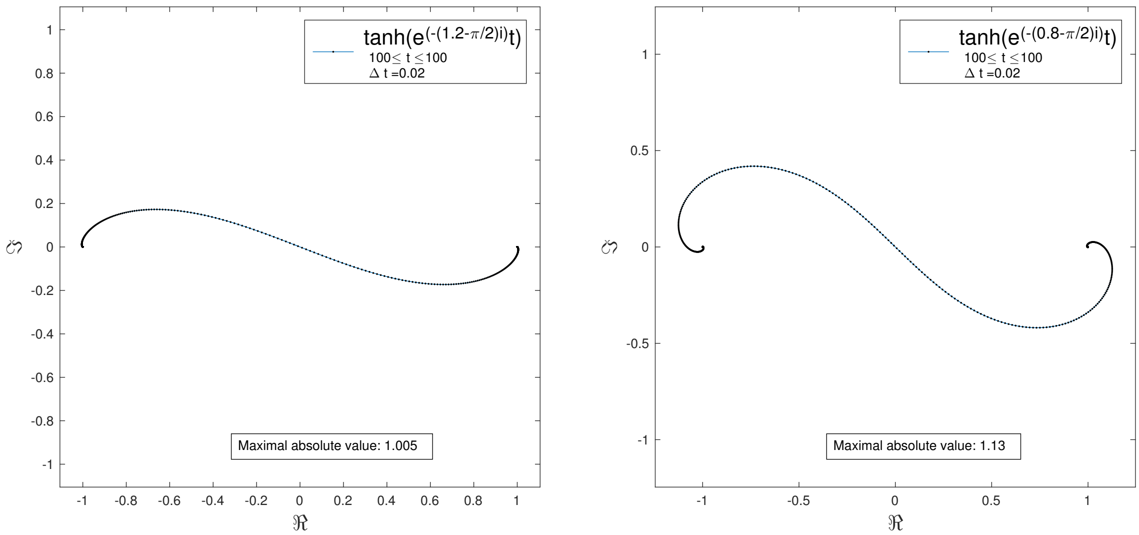

Figure 5: Trajectories for $\phi = 1.2$ and $\phi = 0.8$

If we decrease the value of ϕ to 1.2 and further to 0.8, as plotted in figure 5, the bend becomes bigger and the path even crosses real points on the opposite sides of start and end points before approaching them.

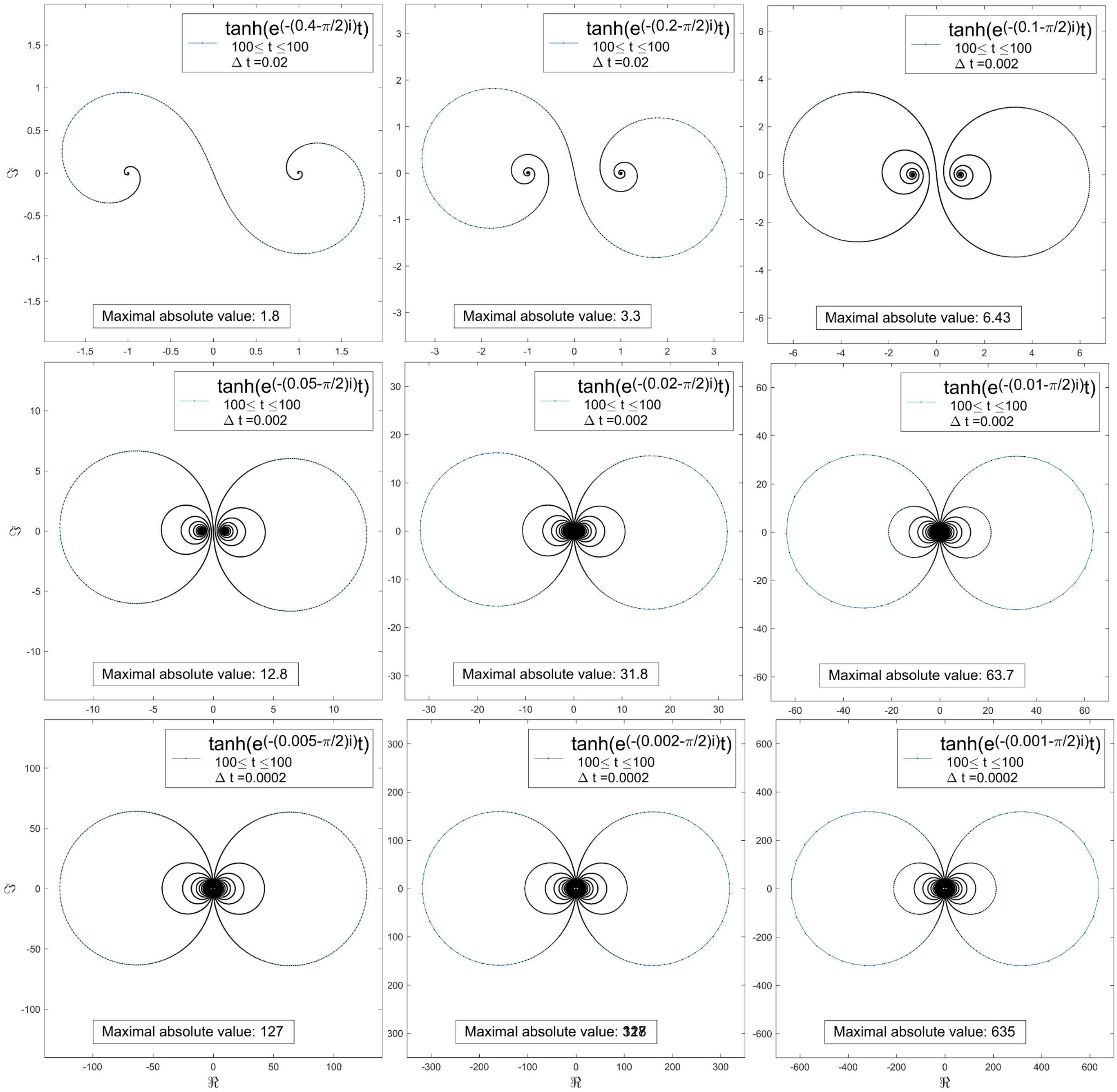

Figure 6: The graphs of $\tanh(e^{(-(\phi-\pi/2)i)}t)$ for $\phi = \begin{matrix} 0.4 & 0.2 & 0.1 \\ 0.05 & 0.02 & 0.01 \\ 0.005 & 0.002 & 0.001 \end{matrix}$

Nine further steps of letting ϕ go towards 0 are shown in figure 6. With decreasing ϕ, the number of windings as well as the extent of the path increase. That is the explanation for the discontinuity at $\phi = 0$: the paths that represent the solutions become larger in an intuitive sense and tend towards being infinitely long with ϕ approaching 0. Hence there is no well-behaved limit path of this sequence that would belong to a similar real-time solution.

Let us try to quantify the apparent divergence. Figure 6 indicates that the path's maximal distance from the origin is continuously increasing with decreasing ϕ. A glance at the numbers suggests that it might be inversely proportional to ϕ.

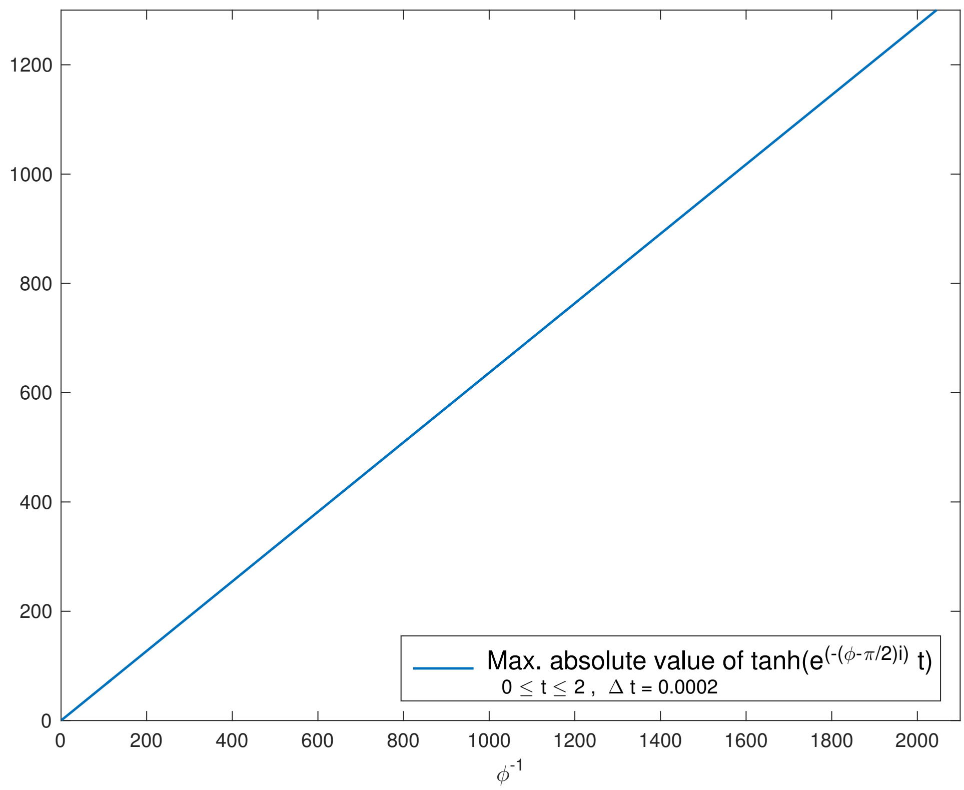

Figure 7: Behaviour of the path's radius with decreasing ϕ

Figure 7 shows a plot of that radius of the path over $\frac{1}{\phi}$, and indeed, we get a straight line with slope 0.63604. That means that the paths are really diverging proportionally to $\frac{1}{\phi}$.

This divergence of the solutions for $\phi \to 0$ is an explanation for the fact that some rotation is needed to receive a path connecting the wells.

9 A Small Complex Phase Arising from Complex Energy

Our goal in this section is to find out which physical occurrences could be responsible for an infinitesimal time axis rotation.

The tangent solution of differential equation 65 for the non-rotated problem is the solution that has zero momentum at the initial and final state. We now examine what we get if we allow small deviations from this constraint.

Multiplying both sides of equation 65 with $\frac{\partial x}{\partial t}$, which is allowed as the solutions won't have finite time spans with $\frac{\partial x}{\partial t} = 0$, extends the equation to

$$-\frac{\partial^2 x}{\partial t^2}\frac{\partial x}{\partial t} = 2\lambda^2 x \frac{\partial x}{\partial t}(x^2 - a^2) \tag{76}$$

which we can integrate to get

$$-\frac{1}{2}\left(\frac{\partial x}{\partial t}\right)^2 = \frac{1}{2}\lambda^2(x^2 - a^2)^2 - \frac{C}{2} \tag{77}$$

with some integration constant $-\frac{C}{2}$. Rewriting this further leads to

$$\frac{\partial x}{\partial t} = \pm\sqrt{-\lambda^2(x^2 - a^2)^2 + C} \tag{78}$$

and

$$\frac{\partial t}{\partial x} = \frac{\pm 1}{\sqrt{C - \lambda^2 (x^2 - a^2)^2}}. \tag{79}$$

We integrate this one again to receive

$$t - t_0 = \int_{t_0}^{t} dt = \int_{0}^{x} \frac{\pm\, dx}{\sqrt{C - \lambda^2 (x^2 - a^2)^2}}. \tag{80}$$

If we simply took $C = 0$, this would give

$$t - t_0 = \pm \frac{1}{i\lambda} \int_{0}^{x} \frac{dx}{x^2 - a^2} = \mp \frac{1}{i\lambda a} \operatorname{artanh}(\frac{x}{a}), \tag{81}$$

or

$$x = \pm a \tanh(i\lambda a(t - t_0)) = \pm ia \tan(\lambda a(t - t_0)), \tag{82}$$

in accordance with section 6.

At this point we want to analyse the role of the integration constant C and to fathom whether there is plausibility for it to be enforcing a small distortion of the solution which is linked to a complex argument. Then it would produce a tunnel path as discussed in the previous sections.

If we regard equation 77 at the starting point $x = -a$ (or, at the end point $x = a$), we get

$$\left(\frac{\partial x}{\partial t}\right)^2 = C \tag{83}$$

Consequently, the physical interpretation of $\frac{C}{2m}$ is the kinetic energy at the beginning of the tunnelling process.

For example, if C is bigger than the potential barrier of $\lambda^2 a^4 = \frac{\kappa}{2m} a^4$, then the expression under the square root in equation 78 is positive for any x. Therefore, the differential equation has a real, i.e. actually classical, solution. Then, as one would suspect, no quantum tunnelling via complex paths is needed to 'jump' from one valley to the other.

Then again for the tunnelling problem we are actually interested in, the particle is initially resting, i.e. $C = 0$ at $x = -a$, which problematically leads to the non-connecting tangent solution. However, since we proved above that even an infinitesimal phase in the equation leads to connecting solutions, we hope to achieve this by assuming an infinitesimal, possibly complex, initial energy C. A physical justification or rather motivation for this idea is that quantum mechanics, which is the framework that is responsible for tunnelling in the first place, demands a non-zero kinetic energy by Heisenberg's uncertainty principle alone.

Letting Wolfram Mathematica 10.3 calculate the integral in equation 80 for $a = 1$, $\lambda = 1$, $\pm = +$, $t_0 = 0$ gives

$$t_C(x) = \int_0^x \frac{dx}{\sqrt{C - (x^2 - 1)^2}} = - \frac{i \sqrt{1 - \frac{x^2}{1-\sqrt{C}}} \sqrt{1 - \frac{x^2}{1+\sqrt{C}}} \, F\left(i \operatorname{arsinh}\left(\sqrt{\frac{-1}{1-\sqrt{C}}} x \right) \middle| \frac{1-\sqrt{C}}{1+\sqrt{C}} \right)}{\sqrt{-\frac{1}{1-\sqrt{C}}} \sqrt{C - (x^2 - 1)^2}} \tag{84}$$

where F is the incomplete elliptic integral of the first kind. For $C \neq 0$, this is quite a complicated term and forming the inverse function $x_C(t)$ does not result in a usable expression. Thus instead of inverting $t_C(x)$, we take the inverse of the connecting phased tanh solution from section 7: In

$$\tanh(e^{-(\phi-\frac{\pi}{2})i}\tau) = x_\phi(\tau) \tag{85}$$

we apply artanh on both sides to get

$$\tau_\phi(x) = e^{(\phi-\frac{\pi}{2})i}\operatorname{artanh}(x). \tag{86}$$

Our hope is that for small energies C and small angles ϕ, the function $t_C(x)$ approaches $\tau_\phi(x)$. Note that we might need to choose the energy C complex. Therefore we let the phase of C fixed as the absolute value goes to 0, just as for ϕ that stays real and positive. To compare the complex-valued functions $t_C(x)$ and $\tau_\phi(x)$, we regard their real and imaginary part separately.

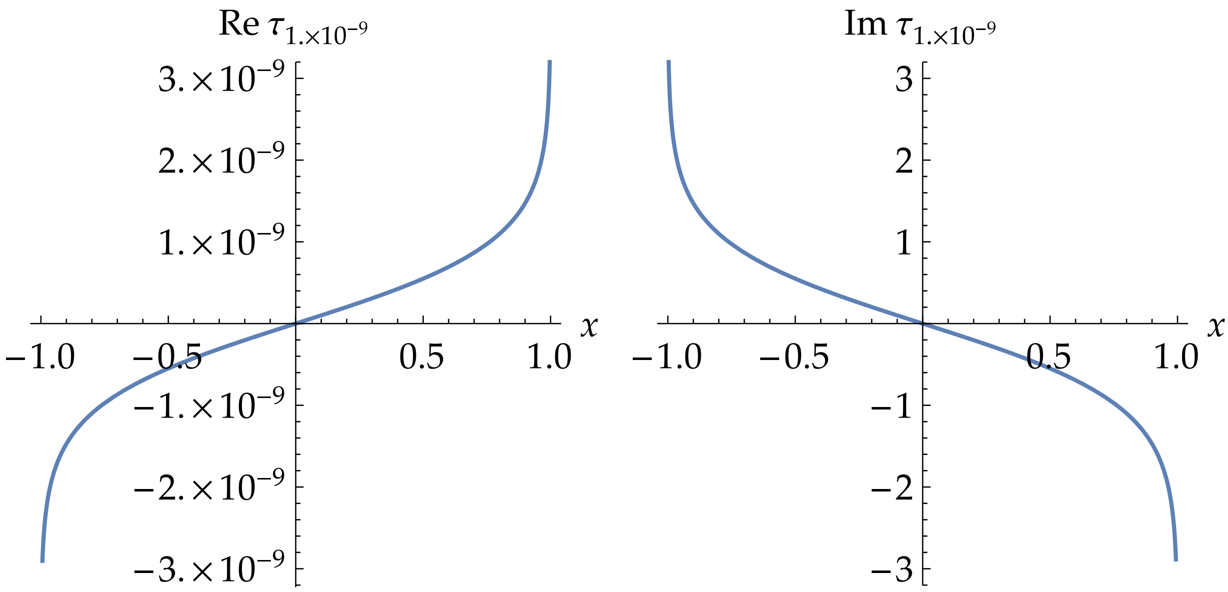

Figure 8: Real and imaginary part of $\tau_{10^{-9}}(x)$

Figure 8 shows Mathematica plots of the real and imaginary part of $\tau_\phi(x)$ over real values of x from -1 to $+1$ for the angle $\phi = 10^{-9}$. As for our tunneling problem, we want the particle to be at -1 at (infinitely negative) real time, the right hand side diagram shows that keeping x real is not working. Actually, we have already seen that the path x must leave the real axis, as illustrated in the plots in section 8. So we settle for purely real time and look at the equation $\tau_\phi(x) = 0$.

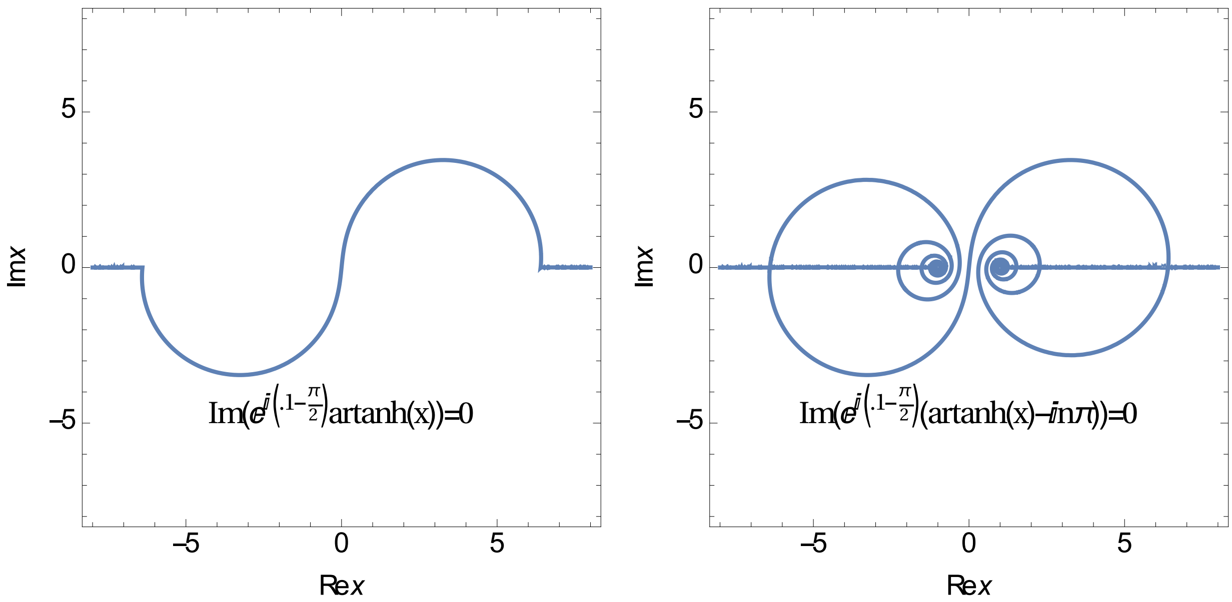

Figure 9: Contour plot of $\tau_{10^{-1}}(x) = 0$ for the standard branch of artanh and for all branches

On the left-hand side of figure 9, we see the points where $\tau_{10^{-1}}(x) = e^{(.1-\frac{\pi}{2})i}\,\text{artanh}(x) = 0$ holds for the standard definition of artanh. The problem here is that the complex inverse function of artanh is not defined on the whole complex plane and thus, artanh is just representing one of its branches. Indeed, there is [cite enc] the identity

$$\text{artanh}(x) = \frac{1}{2}\ln\left(\frac{1+x}{1-x}\right). \tag{87}$$

Thus, for the corresponding areas, the correct function to take is $\mathrm{artanh}(x) + n\pi i$ with an integer n. On the right-hand side of figure 9, we see where the imaginary part of the time vanishes if we allow x to take any branch. It is the anticipated picture that we got without taking the inverse function and drawing the path for real time in equation 6.

For

$$t_C(x) = -\frac{i\sqrt{1-\frac{x^2}{1-\sqrt{C}}}\sqrt{1-\frac{x^2}{1+\sqrt{C}}}\,F\left(i\,\mathrm{arsinh}\left(\sqrt{\frac{-1}{1-\sqrt{C}}}\,x\right)\middle|\frac{1-\sqrt{C}}{1+\sqrt{C}}\right)}{\sqrt{-\frac{1}{1-\sqrt{C}}}\sqrt{C-(x^2-1)^2}} \tag{88}$$

we encounter similar difficulties with different branches.

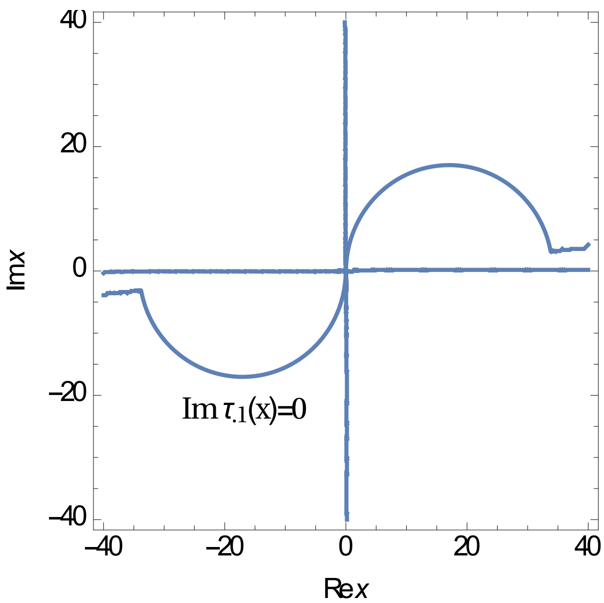

Figure 10: Contour plot of $t_{10^{-1}i}(x) = 0$ for the standard branch

Figure 10 shows the points where this function has vanishing imaginary part. It has a similar shape to the plot for the standard branch of $\tau_{10^{-1}}(x)$. This fact gives us hope that we get a double-spiral connecting $x = -1$ with $x = +1$ as well, when regarding the other branches accordingly. Unfortunately, the higher branches of F and the branch cuts between them get quite complicated. Due to this, it was not possible to produce similar contour plots for those with Mathematica 10.3.

However, $t_C(x)$ is still a good candidate for the tunnelling path. We explore its affinity with $\tau_\phi(x)$ on the real interval between -1 and $+1$ as it is easy to handle here and the identity theorem from complex analysis states that coincidence of the functions here would imply identity. To investigate which phase C should have to make $t_C(x)$ similar to $\tau_\phi(x)$, we first regard the real part of $t_C(x)$. In figure 11 the plots for $C = 10^{-9}$ and $C = 10^{-9}i$ are pictured.

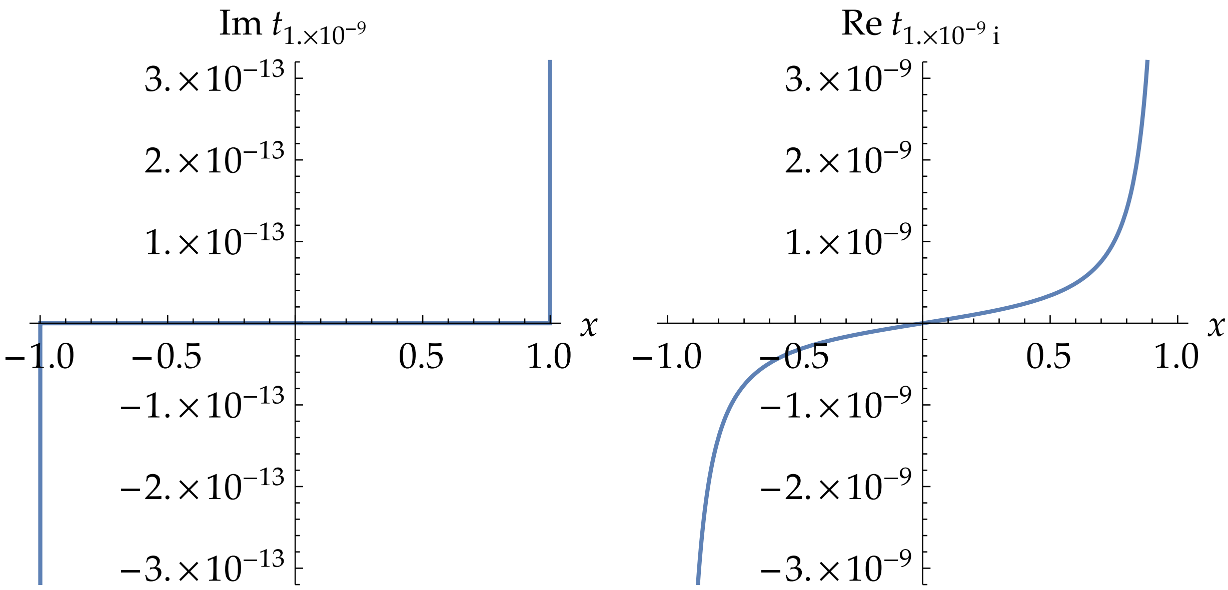

Figure 11: Real part of $t_{10^{-9}}(x)$ and $t_{10^{-9}i}(x)$

While for purely real C, $t_C(x)$ vanishes for $-1 < x < 1$ and thus doesn't coincide with $\tau_\phi(x)$, it very well resembles $\tau_\phi(x)$ if we take it purely imaginary. As playing around with the numbers shows, it does so best if ϕ and $|C|$ are in the same order of magnitude. Even if we do not take the direct resemblance with $\tau_\phi(x)$ into account, we observe that the inverse function of $t_C(x)$ with small imaginary C - its graph is obtained by simply flipping the right-hand plot in figure 11 - does indeed connect $\Re x_C(-\infty) = -1$ with $\Re x_C(\infty) = +1$ and thus fulfills the real part part of being a tunneling process.

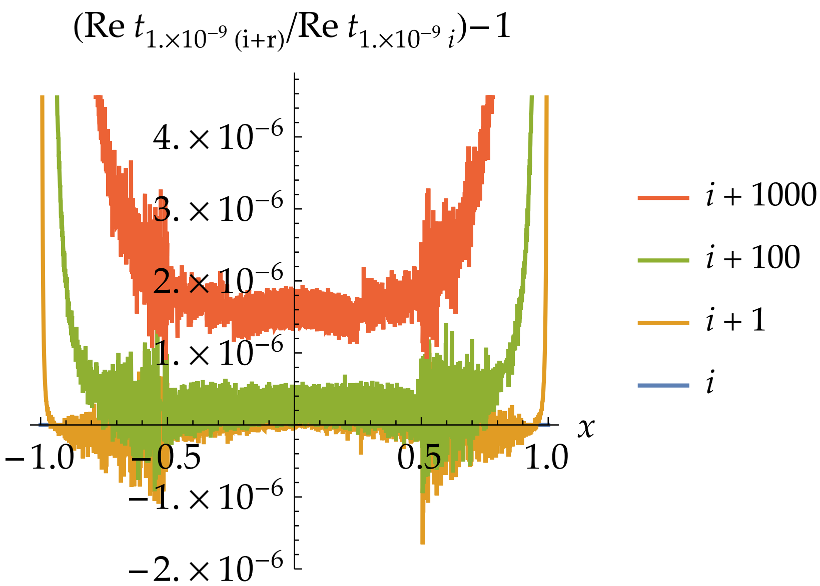

Figure 12: $\frac{\Re t_{10^{-9}(i+r)}}{\Re t_{10^{-9}i}} - 1$ for $r = 0, 1, 100, 1000$

For the question what happens if C has both a real and an imaginary part, we plotted $\frac{\Re t_{10^{-9}(i+r)}}{\Re t_{10^{-9}i}} - 1$ in figure 12 for several real parts r. For $|x|$ not too close to 1, the relative difference to $r = 0$ is small. Thus we are free to choose the phase of C by adding even a comparatively large real part to a very small imaginary part, as long as the absolute value of C still remains small. That is, it might be possible to have C of the form $\epsilon + \epsilon^2 i$ such that in the limit the energy itself is just an infinitesimal phase away from being purely real.

Now we compare the imaginary parts of $t_C(x)$ with small C of different phases to $\tau_\phi(x)$.

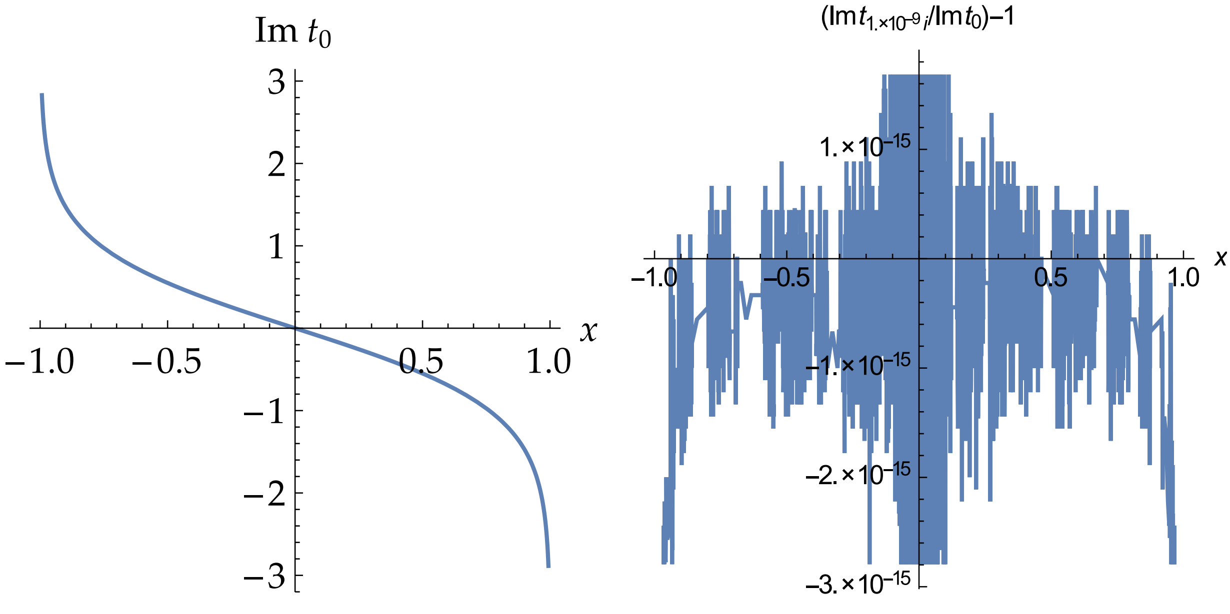

Figure 13: Imaginary part of $t_0(x)$ and $t_{10^{-9}i}(x)$ in comparison

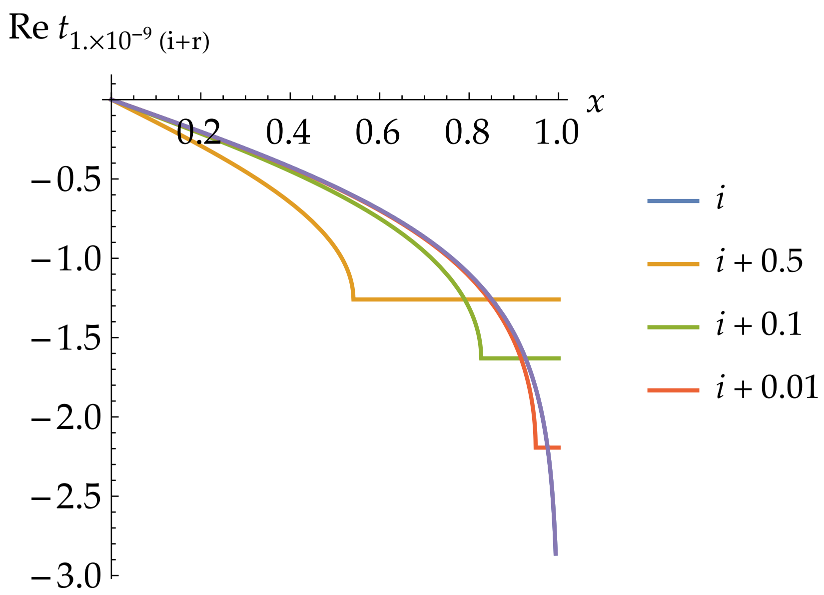

Figure 14: $\Im\, t_{10^{-9}(i+r)}$ for $r = 0, 0.5, 0.1, 0.001$

The plots in figure 13 show the imaginary part of $t_0(x)$ and that it basically doesn't change if we have a small positive imaginary energy C. It is worth noting that if the imaginary part of C is negative, the curve is flipped and thus isn't a solution to the tunneling problem itself, but can be salvaged by assigning $\pm$ to $-$ before equation 84.

Also, a real component of C does not alter the shape of the curve in the $|C| \to 0$ limit, as it then approaches the curve without real part, see figure 14. Again, this well holds in the case $C = \epsilon + \epsilon^2 i$, where the phase angle > 0 becomes arbitrarily small.

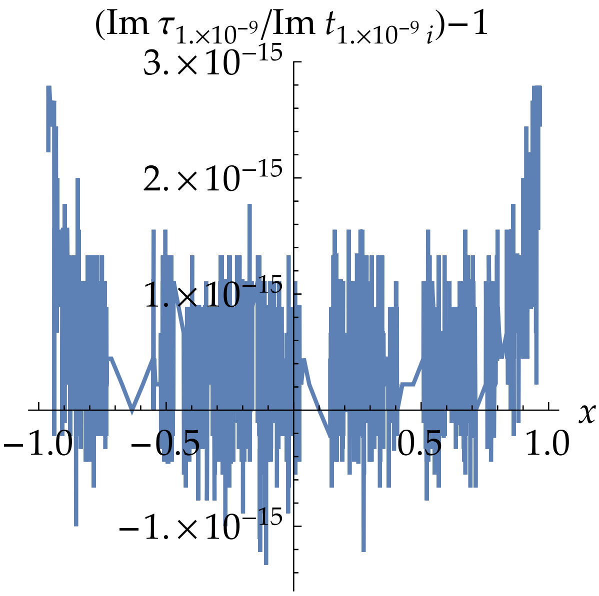

Figure 15: Comparison between the imaginary parts of $t_{10^{-9}i}$ and $\tau_{10^{-9}}$ shows that they are nearly the same

Ultimately, to see how the imaginary parts of t_C and τ_ϕ compare, we visualized their ratio in figure 15 and see that it is very close to 1. Thus, for small $|C|$ with positive imaginary part, the imaginary parts of t_C and τ_ϕ coincide quite precisely.

The bottom line of this comparison is that $t_C(x)$ likely approximates $\tau_\phi(x)$ in the limit of $C, \phi \to 0$ if the energy C has at least a small imaginary part.

As developing a precise technique for analytically examine the function $t_C(x)$'s behaviour for $C \to 0$, we have to content ourselves with this numerical comparison. It indeed suggests that $t_C(x)$ converges towards the $\tau_\phi(x)$-solution. This shifts the problem from explaining the concept of imaginary time towards devising a notion of not purely real energy.

10 Conclusions

With the path integral formalism, the transition amplitude between two states can be expressed as $(a.t_b|{-a}.t_a) = \int \mathcal{D}x\ e^{\frac{i}{\hbar}S[x]}$, for a Hamiltonian that splits into the sum of a kinetic and a potential part which are both time-independent. With $\frac{1}{\hbar}$ huge as it is, it suggests itself to only take into consideration those paths where the other parts of the exponent are large. This notion of largeness is not naturally given in the context of complex numbers. Thus it is helpful to make the exponent purely real. In certain situations, this can be accomplished by a trick called Wick Rotation. This a well established method for solving path integral problems that consists of a 90°-rotation of the time axis in the complex plane.

We showed that for the Hamiltonian describing a particle in a double well potential, the Wick Rotation can be replaced by the rotation by an arbitrarily small angle. The question that arises is why there should be such a thing like complex time in the first place. Our idea to answer this is by assuming small excursions of the system's energy from the real line into the partly imaginary realm of the complex plane. Without those deviations, the situation equals classical mechanics, not allowing tunneling. But as soon as the energy has an imaginary part, a path with minimal action connecting the two wells might be possible; it is to be noted that this position-space path runs far around in the complex plane.

What remains open is to precisely show that the partially imaginary energy leads to a path that exactly connects the bottom points of the well. The problem that we had here is that we ended up with a time function that cannot simply be inverted to a position function, a problem similar to that of the complex logarithm's branching. Another interesting task is to investigate what physics actually happens that leads to imaginary energies. A maybe over-ambitious attempt could be to trace back general quantum mechanical axioms to it. Furthermore, as our considerations take place in the infinite time limit, it might be worth to look for results for finite time spans. And of course there are certainly other potentials and situations where a slight modification of the same contemplations leads to comparable outcomes.

References

[Altland and Simons, 2010] Altland, A. and Simons, B. D. (2010). Condensed matter field theory. Cambridge Univ. Press, Cambridge [u.a.], 2. ed. edition.

[Cherman and Ünsal, 2014] Cherman, A. and Ünsal, M. (2014). Real-Time Feynman Path Integral Realization of Instantons. ArXiv e-prints, 1408.0012.

[Feynman and Brown, 1942] Feynman, R. and Brown, L. (1942). Feynman's Thesis: A New Approach to Quantum Theory. World Scientific.

[Feynman and Hibbs, 1965] Feynman, R. P. and Hibbs, A. R. (1965). Quantum mechanics and path integrals. International series in pure and applied physics. McGraw-Hill, New York [u.a.].

[Kleinert, 1995] Kleinert, H. (1995). Path integrals in quantum mechanics, statistics, and polymer physics. World Scientific, Singapore [u.a.], 2. ed. edition.

[Sudorov, 2001] Sudorov, Y. (2001). Inverse hyperbolic functions. Encyclopaedia of mathematics, Vol. 3, Springer, Dordrecht.

[Tanizaki and Koike, 2014] Tanizaki, Y. and Koike, T. (2014). Real-time Feynman path integral with Picard-Lefschetz theory and its applications to quantum tunneling. Annals of Physics, 351:250–274, 1406.2386.

[Wick, 1954] Wick, G. C. (1954). Properties of bethe-salpeter wave functions. Phys. Rev., 96:1124–1134.