Path integrals in quantum mechanics, Semiclassical approximation

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Abstract

In these notes we present Feynman's path integral formulation of quantum mechanics and we present the semiclassical/WKB approximation in quantum mechanics. The path integral formalism is derived, its equivalence with the Schrödinger's picture is shown, the technique of separable Lagrangians is discussed and the formalism is applied to the statistical physics description of the harmonic oscillator. The WKB approximation is derived, its validity is discussed, connection rules are obtained and they are applied to compute general bound states together with their energies via the derived Born-Sommerfeld rule.

1 Introduction

We consider the description of the non-relativistic 1D dynamics of a quantum particle of mass m [kg] and energy E [J] subject to a time-independent potential $V(x)$ [J], with x [m] the position coordinate and t [s] the time coordinate. In these notes, divided in two parts, we tackle the problem under two different approaches, namely first through a novel quantum mechanical formalism and then through an approximation of the usual quantum description. The former, due to Feynman, allows for a description of quantum phenomena independent of (but equivalent to) the Schrödinger's equation by the means of a functional integral over deterministic paths, hence the name **path integrals**. The latter, due to Wentzel, Kramers and Brilloin, hence the name **WKB**, is an approximation designed to solve the Schrodinger's equation for particle energies much higher than the potential they are interacting with.

2 Path Integrals

2.1 The problem

We want to formulate an alternative physical framework, equivalent to the Schrödinger's picture of quantum phenomena, describing the dynamics of a particle between two space-time points $a = (x_a, t_a)$ and $b = (x_b, t_b)$.

2.2 Classical solution

Classically one identifies the physical path as the one that minimizes the **action** S [Js] functional

$$S[x(t)] = \int_{t_a}^{t_b} L(\dot{x}(t), x(t))\mathrm{d}t, \tag{1}$$

fed by paths $x(t) : [t_a; t_b] \to \mathbb{R}$ with boundary conditions $x(t_a) = x_a, x(t_b) = x_b$, where we integrate over the **Lagrangian** L [J]

$$L(\dot{x}, x) = \frac{m}{2}\dot{x}^2 - V(x) \tag{2}$$

evaluated at the given path. Such a minimizing path is called the **classical path** $\bar{x}(t)$ and it is associated with its **classical action** function $S_{\mathrm{cl}}(b, a) = S[\bar{x}(t)]$. [1, p.26]

2.3 Feynman's solution

In this section we follow Feynman's approach [1, Chapter 1]. Consider, as depicted in figure 1, a source of particles at A and measure the resulting stream of particles reaching screen B, away from A, by the means of a vertically moving detector. In-between A and B place some impenetrable slabs and drill holes in them. Clearly a classical description is insufficient to explain the empirically observed stream of particles producing an interference patter at B. However we notice that before their observed **event** detection at B, particles starting from A have a finite amount of possible paths, or unobserved **methods**, available to them to reach

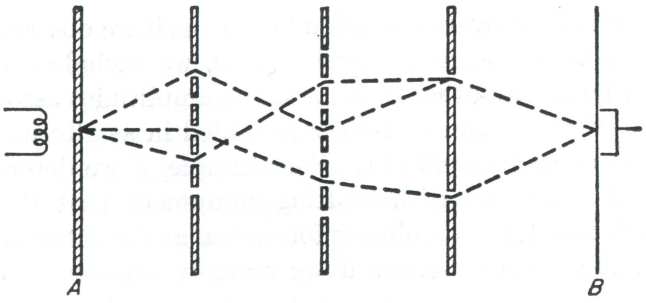

Figure 1: Feynman's historical thought experiment of particles emitted at A reaching a screen B after interacting with obstacles. Adapted from [1].

screen B. We postulate that each method j is associated to an **amplitude** $\phi_j \in \mathbb{C}$ and that overall methods interfere with each other producing a **total amplitude** of the whole event

$$\phi = \sum_j \phi_j. \tag{3}$$

The observed detection probability is then postulated to be proportional to $P = |\phi|^2 \in \mathbb{R}$. The number of slabs and the number of holes in them is arbitrary, therefore we take the limit of infinitely many slabs with infinitely many holes to obtain a constrained vacuum where at each horizontal position particles are forced to pick a vertical one, thus following a continuous path. In this limit the finite amount of methods becomes the infinite amount of possible paths $x(t)$ between space-time points a and b, as in figure 2. If we postulate the **transition amplitude** of a path $x(t)$ to be

$$\phi[x(t)] \sim \exp\left(\frac{i}{\hbar} S[x(t)]\right) \tag{4}$$

then the **total transition amplitude** is

$$\begin{aligned} K(b,a) &:= \sum_{\substack{\text{all paths} \\ a \to b}} \phi[x(t)] \\ &=: \int \exp\left(\frac{i}{\hbar} S[x(t)]\right) \mathrm{D}x(t). \end{aligned} \tag{5}$$

The last equality is called the **path integral** and it suggests a functional integration over varying paths, captured in the measure $\mathrm{D}x(t)$. The meaning of the measure is understood by applying many

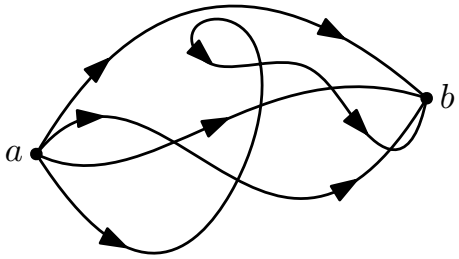

Figure 2: Limiting result of figure 1 as the number of slabs and holes in them goes to infinity.

times the **composition rule**[1] [1, p.37]

$$K(b,a) = \int K(b,c)K(c,a)\mathrm{d}x_c, \tag{6}$$

which is true since any path $a \to b$ can be broken into two pieces $a \to c$ and $c \to b$. Notice how matching of derivatives at c is unnecessary as all paths, even the matching one, must be considered. Then, breaking the path into N pieces each of **time step** duration $\varepsilon = (t_b - t_a)/N$ we get [1, p.38]

$$K(b,a) = \lim_{\varepsilon \to 0} \int \mathrm{d}x_1 \cdots \int \mathrm{d}x_{N-1} \prod_{i=1}^{N} K(i, i-1), \tag{7}$$

with $(b,a) \equiv (N,0)$ and therefore, in the limit $\varepsilon \to 0$, $\mathrm{d}x_1 \cdots \mathrm{d}x_{N-1} \to \mathrm{D}x(t)$ represents the variation of the discretized path $(x_1, \ldots, x_{N-1}) \to x(t)$.

How come the infinite (5) sum converges? Consider paths varying around $\bar{x}(t)$: for paths sufficiently close to $\bar{x}(t)$ then $|S[x(t)] - S_{\mathrm{cl}}(b,a)| < \pi\hbar$ and the amplitudes interfere constructively. However for paths sufficiently away from $\bar{x}(t)$ then $|S[x(t)] - S_{\mathrm{cl}}(b,a)| > \pi\hbar$ and the phase starts to violently spin, therefore amplitudes interfere destructively. Overall only paths $x(t) \approx \bar{x}(t)$ up to the quantum scale $\pi\hbar$ contribute: in the classical limit $\hbar \to 0$ indeed only $\bar{x}(t)$ contributes. [1, p.29-30]

2.4 Schrödinger implies Feynman

Following [2, Section 2.1], we show that the Schrödinger's picture implies the path integral representation of quantum phenomena. Given an initial state $|\psi(t_a)\rangle$, its time evolution $|\psi(t_b)\rangle$ is obtained by applying the **time evolution operator**

$$\hat{U}(t_b, t_a) = \exp\left(-\frac{i}{\hbar}(t_b - t_a)\hat{H}\right), \tag{8}$$

[1] In these notes, by convention, a regular integral without bounds is understood as an integral over $\mathbb{R}$.

implied by the Schrödinger's equation. Hence

$$\psi(x_b,t_b) = \langle x_b \,|\, \psi(t_b)\rangle = \left\langle x_b \middle| \hat{U}(t_b,t_a) \middle| \psi(t_a)\right\rangle = \int \mathrm{d}x_a \left\langle x_b \middle| \hat{U}(t_b,t_a) \middle| x_a\right\rangle \psi(x_a,t_a). \tag{9}$$

If we split the Hamiltonian into a kinetic $\hat{T}$ and a potential $\hat{V}$ part, generally not commuting $[\hat{T},\hat{V}] \neq 0$, then by applying **Trotter's formula** [2, p.93]

$$e^{\hat{T}+\hat{V}} = \lim_{N\to\infty} \prod_{k=1}^{N} e^{\hat{T}/N} e^{\hat{V}/N} \tag{10}$$

the above sandwich containing $\hat{H} = T(\hat{p}) + V(\hat{x})$ becomes (omitting the limit $N \to \infty$)

$$\left\langle x_b \middle| \hat{U}(t_b,t_a) \middle| x_a\right\rangle = \left\langle x_b \middle| \prod_{k=1}^{N} e^{-i\varepsilon\hat{T}/\hbar} e^{-i\varepsilon\hat{V}/\hbar} \middle| x_a\right\rangle = \prod_{k=1}^{N-1}\left(\int \mathrm{d}x_k\right) \prod_{k=1}^{N} \left\langle x_k \middle| e^{-i\varepsilon\hat{T}/\hbar} e^{-i\varepsilon\hat{V}/\hbar} \middle| x_{k-1}\right\rangle, \tag{11}$$

where $N-1$ identity operators in position space were inserted between the N factors and where we identify $(x_b,x_a) \equiv (x_N,x_0)$. The N sandwiches can be easily evaluated with a change of basis $|x\rangle \to |p\rangle$, the **position-momentum sandwich** $\langle x|p\rangle = e^{ipx/\hbar}/\sqrt{2\pi\hbar}$ and a Gaussian integration[2], after which one is left with

$$\left\langle x_b \middle| \hat{U}(t_b,t_a) \middle| x_a\right\rangle = \lim_{N\to\infty} \int \mathrm{d}x_1 \cdots \int \mathrm{d}x_{N-1} \, A^N \exp\left(\varepsilon \frac{i}{\hbar} \sum_{k=1}^{N} \left[\frac{m}{2}\left(\frac{x_k - x_{k-1}}{\varepsilon}\right)^2 - V(x_{k-1})\right]\right), \tag{12}$$

where the constant $A := \sqrt{m/(2\pi i\hbar\varepsilon)}$ has been defined. By recognising in (12) the Riemann sum of (1) in the exponential, the metric $\mathrm{D}x(t)$ and by absorbing A^N in the amplitude, in accordance with (4), one arrives at the path integral

$$\left\langle x_b \middle| \hat{U}(t_b,t_a) \middle| x_a\right\rangle = \int \exp\left(\frac{i}{\hbar} S[x(t)]\right) \mathrm{D}x(t), \tag{13}$$

which is the desired result. Overall, by (9), the path integral is the integral **kernel** that time-evolves wavefunctions [1, p.57]

$$\psi(x_b,t_b) = \int K(b,a)\psi(x_a,t_a)\mathrm{d}x_a \tag{14}$$

[2]See Appendix A.

and hence, comparing with (6), wavefunctions $\psi(x_b,t_b)$ can be seen as kernels $K(b,a)$ for which the initial transition point a was forgotten [1, p.57]. Indeed, by injecting (14) into the Schrödinger's equation with $(x,t) \equiv (x_b,t_b)$ and by selecting $\psi(x'_a,t_a) = \delta(x'_a - x_a)$ one effectively obtains that the kernel is a solution of the Schrödinger's equation [1, p.81]

$$i\hbar\frac{\partial K}{\partial t_b}(b,a) = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_b^2} + V(x_b)\right] K(b,a). \tag{15}$$

The **normalization of the path integral**, however, takes a different form [1, p.83]:

$$\forall x_a : 1 = \iint \mathrm{d}x_c \mathrm{d}x_b \, K^*(c,b)K(c,a), \tag{16}$$

where $t_c > t_a = t_b$, obtained from the identity [3]

$$1 = \int \mathrm{d}x_b \left\langle x_b \middle| \hat{U}^\dagger(t_c,t_b)\hat{U}(t_c,t_a) \middle| x_a\right\rangle. \tag{17}$$

As a final remark, by inserting two identity operators in energy eigenstates basis $|n\rangle$ (they satisfy $\hat{H}|n\rangle = E_n|n\rangle$ for $n \in \mathbb{N}$) in (13) and by denoting $\phi_n(x) = \langle x|n\rangle$ one obtains [1, p.88]

$$K(b,a) = \sum_{n=0}^{\infty} \phi_n(x_b)\phi_n^*(x_a) e^{-i(t_b-t_a)E_n/\hbar}. \tag{18}$$

2.5 Feynman implies Schrödinger

Following [1, Section 4.1], we show the inverse direction of the preceding section. Denote $(x_a,t_a) \equiv (y,t), (x_b,t_b) \equiv (x,t+\varepsilon)$ for $\varepsilon \ll 1$ and, in sight of the antecedent discussion, apply (6) to obtain

$$\psi(x,t+\varepsilon) \sim \int \mathrm{d}y \, \psi(y,t) e^{\frac{im}{2\hbar\varepsilon}(x-y)^2} e^{-\frac{i\varepsilon}{\hbar}V\left(\frac{x+y}{2},t\right)}, \tag{19}$$

where (1) was discretized. Because of the first exponential, only terms $y = x+\eta$ with $\eta \ll 1$ will constructively contribute to the integral, hence by changing variables

$$\psi(x,t) + \varepsilon\frac{\partial\psi}{\partial t}(x,t) \sim \int \mathrm{d}\eta \, \psi(y,t) \exp\left(\frac{im\eta^2}{2\hbar\varepsilon}\right) \left(1 - \frac{i\varepsilon}{\hbar}V(x,t)\right)\left(\psi(x,t) + \frac{\eta^2}{2}\frac{\partial^2\psi}{\partial x^2}(x,t)\right), \tag{20}$$

where we expanded all quantities up to order ε and $\eta^2 \sim \varepsilon$ (due to the very same first exponential).

The integration can now be performed and we end up with

$$\psi(x,t)+\varepsilon\frac{\partial\psi}{\partial t}(x,t)=A\sqrt{\frac{2\pi i\hbar\varepsilon}{m}}\left(\psi(x,t)+\frac{i\hbar\varepsilon}{2m}\frac{\partial^2\psi}{\partial x^2}(x,t)-\frac{i\varepsilon}{\hbar}V(x,t)\psi(x,t)\right), \tag{21}$$

where we replaced the proportionality with the equality and some unknown constant $A\in\mathbb{C}$. In order to obtain a finite quantity when $\varepsilon\to 0$ it must be $A=\sqrt{m/(2\pi i\hbar\varepsilon)}$, as expected. By cancelling the square root with A and by rearranging the above equation we obtain the Schrödinger's equation, which is the desired result.

2.6 Separable Lagrangians

Equation (12) gives us a cumbersome definition of the path integral because it requires $N-1$ integrations: we want to avoid such laborious work [4]. To this end consider **separable Lagrangians** which, upon decomposition $x(t)=\bar{x}(t)+y(t)$ with $y(t_a)=y(t_b)=0$ [1, p.59] as in figure 3, satisfy [4]

$$S[x(t)]=S_{\text{cl}}(b,a)+R[y(t)] \tag{22}$$

for some functional R. In such a case the path integral becomes [4]

$$K(b,a)=F(t_b,t_a)\exp\left(\frac{i}{\hbar}S_{\text{cl}}(b,a)\right) \tag{23}$$

and, since $F(t_b,t_a):=K(0,0)$, by time translational symmetry $F(t_b,t_a)=F(T)$ with $T=t_b-t_a$ [1, p.61]. If a Lagrangian is exactly separable then the difficulty of the $N-1$ integrations is substituted by the determination of $F(T)$ [1, p.62], for example using (16). It is worth noting that $F(T)$ is actually not so important, as frequently only ratios of kernels are actually needed and hence the factors $F(T)$ cancel out [4].

An example of separable Lagrangian is the class of **quadratic Lagrangians**

$$L(\dot{x},x)=a\dot{x}^2+b\dot{x}x+cx^2+d\dot{x}+ex+f \tag{24}$$

with $a,b,c,d,e,f\in\mathbb{R}$ [1, p.58]. A laborious, but trivial, work of partial integrations can show that for them indeed [1, p.60]

$$S[x(t)]=S_{\text{cl}}(b,a)+\int_{t_a}^{t_b}\left(a\dot{y}^2+b\dot{y}y+cy^2\right)\mathrm{d}t. \tag{25}$$

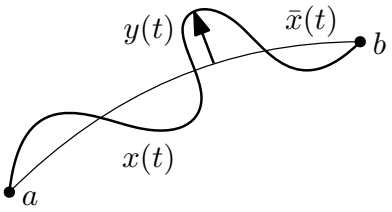

Figure 3: Decomposition of a generic path $x(t)$ from a to b by the means of a generic variation $y(t)$ around the fixed classical path $\bar{x}(t)$.

This implies that any non-exactly separable Lagrangian can be approximately separable by Taylor expanding the potential in it and bringing the former in a quadratic form [1, p.62].

2.7 Statistical Physics

The path integral formalism can be of great help in the computation of the **partition function** $Z=\text{Tr}(\hat{\rho})$ of thermodynamical systems of Hamiltonian $\hat{H}$ described in the **canonical ensemble**, whose **density matrix** is given by $\hat{\rho}=e^{-\beta\hat{H}}$, where $\beta\,[\text{J}^{-1}]$ is the (fixed) inverse temperature [4]. Indeed, by computing

$$Z=\text{Tr}(\hat{\rho})=\int\mathrm{d}x'\,\langle x'|e^{-\beta\hat{H}}|x'\rangle \tag{26}$$

we observe that the matrix element is equivalent to (13) provided the following identifications: **periodic boundary conditions** $x_a=x_b=x'$ and the **time-temperature identification** $iT=\beta\hbar$ [4]. In particular, being $\beta\hbar\in\mathbb{R}$, the latter implies the presence of a **Wick rotation** $t\to it=:\tau$ to **imaginary time** $\tau\in\mathbb{R}$, therefore t is now a negative imaginary number and $\beta\hbar=i(t_b-t_a)=\tau_b-\tau_a$, as illustrated in figure 4 [4]. In order to link the partition function with the path integral, it is standard practice in the literature (see for example [1,

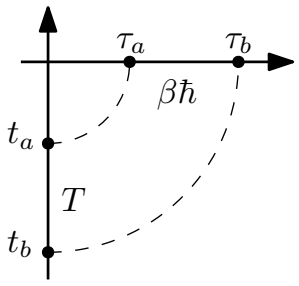

Figure 4: Wick rotation in the complex plane $\mathbb{C}$.

p.275] or [4]) to perform a not-so rigorous change of imaginary-to-real variable $t \to it = \tau$ in (1). In this report we instead apply a more rigorous argument of our own invention. First, analytically extend paths $x(z)$ in the complex plane of times $z \in \mathbb{C}$ and demand the former to be rotationally i-periodic $x(iz) = x(z)$. This is because we want the same dynamics on both the imaginary and real axis $x(t) = x(\tau)$. Then, referring to figure 4, compute the complex integral[3] reinterpretation of (1), where $\dot{x}(z) = (\mathrm{d}x/\mathrm{d}z)(z)$, along the straight line path $t_a \to t_b$ by parametrizing $z(\lambda) = -i\lambda$ for $\lambda \in [\tau_a; \tau_b] \subset \mathbb{R}$. The action then becomes

$$\begin{aligned} S[x(t)] &= \int_{t_a \to t_b} \mathrm{d}z \left[\frac{m}{2} \left(\frac{\mathrm{d}x}{\mathrm{d}z}(z) \right)^2 - V(x(z)) \right] \\ &= \int_{\tau_a}^{\tau_b} \mathrm{d}\lambda \, (-i) \left[\frac{m}{2} \left(\frac{\mathrm{d}x}{\mathrm{d}z}(-i\lambda) \right)^2 - V(x(-i\lambda)) \right] \\ &= -i \int_{\tau_a}^{\tau_b} \mathrm{d}\lambda \left[\frac{m}{2} \left(i \frac{\mathrm{d}}{\mathrm{d}\lambda} x(-i\lambda) \right)^2 - V(x(-i\lambda)) \right] \\ &= i \int_{\tau_a \to \tau_b} \mathrm{d}z \left[\frac{m}{2} \left(\frac{\mathrm{d}x}{\mathrm{d}z}(z) \right)^2 + V(x(z)) \right] \\ &= i S_E[x(\tau)], \end{aligned} \tag{27}$$

where the second line follows by definition, in the third line we apply the chain rule, in the forth line we apply the i-periodicity and in the last equality we define the **Euclidean action** S_E [Js] [4]

$$S_E[x(\tau)] = \int_{\tau_a}^{\tau_b} H(\dot{x}(\tau), x(\tau)) \mathrm{d}\tau, \tag{28}$$

which, we recognise, integrates over the **classical Hamiltonian** H [J]

$$H(\dot{x}, x) = \frac{m}{2} \dot{x}^2 + V(x). \tag{29}$$

Notice how the measure $\mathrm{d}t$ and therefore also $\mathrm{d}\tau$ is just a dummy renaming of $\mathrm{d}z$. Eventually the above computation shows the relationship between the two actions to be $S[x(t)] = iS_E[x(\tau)]$ and therefore, stitching everything together, the link between the partition function and the **Euclidean path integral** is given by [4]

$$Z = \int \mathrm{d}x' \int \exp\left(-\frac{1}{\hbar} S_E[x(\tau)] \right) \mathrm{D}x(\tau). \tag{30}$$

[3] See Appendix B.

In practice, in order to compute the matrix element, it is sufficient to perform the time-temperature substitution $T = -i\beta\hbar$ in $K(b, a)$ [4].

2.8 Typical examples

For the **free particle** $V \equiv 0$ the classical action is trivially [1, p.27]

$$S_{\mathrm{cl}}(b, a) = \frac{m}{2} \frac{(x_b - x_a)^2}{t_b - t_a} \tag{31}$$

and, since its Lagrangian is separable, using (23)

$$K(b, a) = \sqrt{\frac{m}{2\pi i\hbar T}} \exp\left(\frac{im(x_b - x_a)^2}{2\hbar(t_b - t_a)} \right), \tag{32}$$

where its $F(t)$ was found by normalization (16) [4].

For the **harmonic oscillator** $V(x) = m\omega^2 x^2/2$, with frequency ω [s^{-1}], one finds [1, p.28]

$$S_{\mathrm{cl}}(b, a) = \frac{m\omega}{2\sin(\omega T)} \Big[(x_a^2 + x_b^2) \cos(\omega T) - 2x_a x_b \Big] \tag{33}$$

and, likewise [4],

$$K(b, a) = \sqrt{\frac{m\omega}{2\pi i\hbar \sin(\omega T)}} \exp\left\{ \frac{im\omega}{2\hbar \sin(\omega T)} \Big[(x_a^2 + x_b^2) \cos(\omega T) - 2x_a x_b \Big] \right\}. \tag{34}$$

Notice how this kernel is equivalent to the free particle one by letting $\omega \to 0$. We now apply the concepts of the precedent section. By substituting[4] $T = -i\beta\hbar$ and requiring $x_a = x_b = x$ above one obtains [4]

$$\begin{aligned} \langle x | e^{-\beta \hat{H}} | x \rangle &= \sqrt{\frac{m\omega}{2\pi\hbar \sinh(\beta\hbar\omega)}} \\ &\exp\left(-\frac{m\omega x^2}{\hbar \sinh(\beta\hbar\omega)} \Big[\cosh(\beta\hbar\omega) - 1 \Big] \right) \end{aligned} \tag{35}$$

which, integrated, yields [4]

$$\begin{aligned} Z &= \int \mathrm{d}x \, \langle x | e^{-\beta \hat{H}} | x \rangle = \frac{e^{-\beta\hbar\omega/2}}{1 - e^{-\beta\hbar\omega}} \\ &= \sum_{n=0}^{\infty} \exp\left(-\beta\hbar\omega \left(n + \frac{1}{2} \right) \right) \\ &= \sum_{n=0}^{\infty} e^{-\beta E_n} = \sum_n \langle n | e^{-\beta \hat{H}} | n \rangle = \mathrm{Tr}(\hat{\rho}), \end{aligned} \tag{36}$$

where $E_n = \hbar\omega(n + 1/2)$ are the eigenenergies of the energy eigenstates, giving us the expected harmonic oscillator spectrum.

[4] See Appendix C.

3 WKB approximation

3.1 The problem

We want to approximately solve the **time-independent Schrödinger's equation**

$$\left(-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}+V(x)\right)\psi(x)=E\psi(x). \tag{37}$$

To this end we associate semiclassical quantities to the particle [5]: the **local momentum** $p\,[\mathrm{kg}\cdot\mathrm{m/s}]$

$$p(x):=\sqrt{2m[E-V(x)]} \tag{38}$$

and the **local de Broglie's wavelength** $\lambda\,[\mathrm{m}]$

$$\lambda(x):=2\pi\hbar/p(x), \tag{39}$$

connected to $p(x)$ by the means of the **local wavevector** $k(x)=p(x)/\hbar$. We'll call a **turning point** any solution of $V(x)=E$ [5].

3.2 Derivation

We follow [5]. We rewrite (37) in the form

$$\left[\hbar^2\frac{\mathrm{d}^2}{\mathrm{d}x^2}+p(x)^2\right]\psi(x)=0 \tag{40}$$

and propose the ansatz $\psi(x)=e^{iS(x)/\hbar}$ with $S(x)\,[\mathrm{Js}]$ the so-called **eikonal**. This leads to

$$\left(\frac{\mathrm{d}S}{\mathrm{d}x}\right)^2-i\hbar\frac{\mathrm{d}^2S}{\mathrm{d}x^2}=p(x)^2, \tag{41}$$

which can be solved thanks to the **semiclassical expansion** of the eikonal

$$S(x)=\sum_{j=0}^{\infty}\hbar^j S_j(x), \tag{42}$$

where j is called the **order** and the powers of $\hbar$ play the role of order bookkeeping. Injecting (42) into (40) and grouping together terms of same order gives us at order $j=0$

$$\left(\frac{\mathrm{d}S_0}{\mathrm{d}x}\right)^2=p(x)^2, \tag{43}$$

solved by the two solutions

$$S_0(x)=\pm\int_{x_0}^{x}p(y)\mathrm{d}y, \tag{44}$$

with x_0 such that $S_0(x_0)=0$; at order $j=1$

$$2\frac{\mathrm{d}S_0}{\mathrm{d}x}\frac{\mathrm{d}S_1}{\mathrm{d}x}=i\frac{\mathrm{d}^2S_0}{\mathrm{d}x^2}, \tag{45}$$

solved, using S_0, by

$$S_1(x)=\frac{1}{i}\ln\left(\frac{1}{\sqrt{p(x)}}\right)+\text{const}; \tag{46}$$

and at order $j=2$, using S_0 and S_1,

$$2\frac{\mathrm{d}S_0}{\mathrm{d}x}\frac{\mathrm{d}S_2}{\mathrm{d}x}=-\left(\frac{\mathrm{d}S_1}{\mathrm{d}x}\right)^2+i\frac{\mathrm{d}^2S_1}{\mathrm{d}x^2}. \tag{47}$$

A recurrence relation for generic j can be derived but since we'll truncate (42) at order $j=2$ we only need to estimate the error on the S_2 solution:

$$S_2(x)=\int_{x_0}^{x}\frac{3p'(y)^2-2p(y)p''(y)}{8p(y)^3}\mathrm{d}y=O\left(\frac{\lambda}{L}\right), \tag{48}$$

where we count a contribution of $L\,[\mathrm{m}]$, the **characteristic length** over which $V(x)$ varies, for each integration, a contribution of $1/L$ for each differentiation and a contribution of $p\sim k\sim 1/\lambda$ for each local momentum. The asymptotic behaviour of S_2 suggests that the WKB approximation is accurate if for the wavefunction $\lambda\ll L$: that is [5]

$$\left|\frac{\mathrm{d}\lambda}{\mathrm{d}x}\right|=2\pi\hbar\left|\frac{p'(x)}{p(x)}\right|\sim\lambda\left|\frac{V'(x)}{E-V(x)}\right|\ll 1, \tag{49}$$

meaning that the WKB approximation breaks down close to turning points. Overall, stitching S_1 and S_2 back in the ansatz, we obtain the (unnormalized) **WKB wavefunctions** [5]

$$\psi_\pm(x)=\frac{1}{\sqrt{p(x)}}\exp\left(\pm\frac{i}{\hbar}\int_{x_0}^{x}p(y)\mathrm{d}y\right). \tag{50}$$

Notice how the approximation explodes to infinity at turning points due to the denominator. For $E>V(x)$ it is $p(x)^2>0$ and (50) is valid, however for $E<V(x)$ it is $p(x)^2<0$ so we must rewrite $p(x)=\pm i|p(x)|$ and the WKB wavefunctions becomes [5]

$$\psi_\pm(x)=\frac{1}{\sqrt{|p(x)|}}\exp\left(\pm\frac{1}{\hbar}\int_{x_0}^{x}|p(y)|\mathrm{d}y\right). \tag{51}$$

For a constant potential, hence a constant $p(y)$, the integrations are trivial and one readily obtains the usual wave and exponential solutions [4].

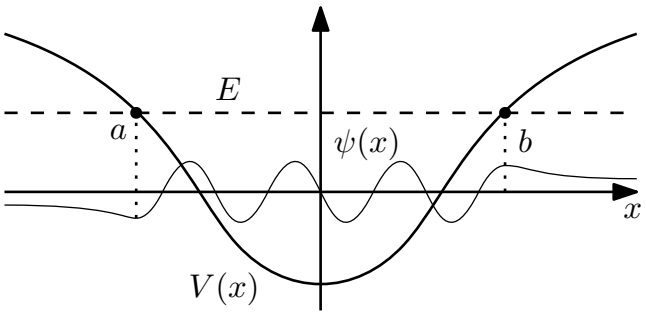

Figure 5: Bound state $\psi(x)$ in a binding potential $V(x)$ confined between tuning points a, b. The qualitative behaviour of $\psi(x)$ is shown.

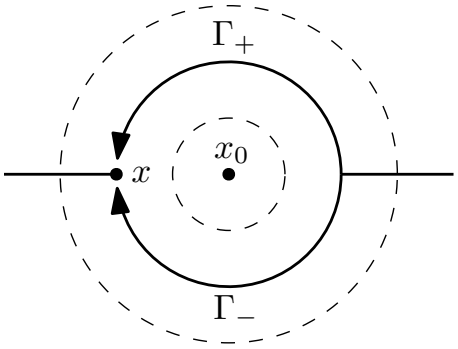

Figure 6: Contouring of the turning point x_0 in the complex plane $\mathbb{C}$ by the means of paths $\Gamma_\pm$ starting from and ending on the real line.

3.3 Connection rules

We want to compute the bound states of a generic binding potential for which exactly two turning points $a < b$ exist, dividing space in a classically allowed $x \in [a;b]$ and forbidden $x \notin [a;b]$ region [5], as depicted in figure 5. In the allowed region $E > V(x)$ therefore $\psi(x)$ is a superposition of (50), namely [6, p.161]

$$\begin{aligned}\psi(x) = &\frac{C_1}{\sqrt{p(x)}} \exp\left(\frac{i}{\hbar}\int_b^x p(y)\mathrm{d}y\right) \\ &+ \frac{C_2}{\sqrt{p(x)}} \exp\left(-\frac{i}{\hbar}\int_b^x p(y)\mathrm{d}y\right)\end{aligned} \tag{52}$$

for some $C_1, C_2 \in \mathbb{C}$. In the forbidden region $E < V(x)$ hence one must use (51), but since we must ensure the wavefunction to be normalizable $\psi(x) \in L^2(\mathbb{R})$, we select the solution that exponentially decays at $x \to \pm\infty$ [5]. Focusing from now on on turning point $x_0 = b$, in particular requiring $V'(x_0) > 0$, it is [6]

$$\psi(x) = \frac{C}{\sqrt{|p(x)|}} \exp\left(-\frac{1}{\hbar}\int_b^x |p(y)|\mathrm{d}y\right) \tag{53}$$

for some $C \in \mathbb{C}$. Our goal is now to find the matching relationships between C_1, C_2, C in order to stitch together the two regimes. However we can't just equate the solutions at x_0 since due to the criterion (49) we must stay away from x_0 [5]. The way out is to analytically continue all functions of $x \in \mathbb{R} \to \mathbb{C}$ and take advantage of the extra dimension in the complex plane to contour x_0 in a clockwise Γ_- or anti-clockwise Γ_+ path [5], as in figure 6. To simplify computations we linearly approximate the difference [5]

$$\begin{aligned}E - V(x) &= E - V\left((x - x_0) + x_0\right) \\ &\approx E - \left[V(x_0) + V'(x_0)(x - x_0)\right] \\ &= V'(x_0)(x_0 - x)\end{aligned} \tag{54}$$

which implies

$$\begin{aligned}|p(x)| &= \sqrt{2mV'(x_0)}\sqrt{x - x_0} \\ &= \sqrt{2mV'(x_0)|x - x_0|}e^{i\arg(x-x_0)/2} \\ &= \pm ip(x),\end{aligned} \tag{55}$$

where we used that any complex number $z \in \mathbb{C}$ can be written in the form $z = |z|e^{i\arg(z)}$ and picking $\Gamma_\pm$ it is $\arg(x - x_0) = \pm\pi$. The inner dashed circle of figure 6 is the region where the WKB approximation breaks down, while the outer dashed circle is the region where (54) is valid: $\Gamma_\pm$ must therefore pass in between the two [5]. We can now take solution (53) and transport it along $\Gamma_\pm$, from $x > x_0$ to $x < x_0$, and observe that since $|p(x)| \to \pm ip(x)$ then (53) falls in one of the two summands in superposition (52), allowing for the identification [6, p.162]

$$\begin{cases} C_1 = Ce^{i\pi/4} \\ C_2 = Ce^{-i\pi/4} \end{cases} \tag{56}$$

Finally we can restate (52) as [5]

$$\psi(x) = \frac{2C}{\sqrt{p(x)}} \cos\left(\int_b^x \frac{p(y)}{\hbar}\mathrm{d}y + \frac{\pi}{4}\right), \tag{57}$$

where we notice that the two important numbers here are the factor of 2 in front of C and the $\pi/4$ phase shift. The analysis for turning point a is analogous and it leads to almost the same wavefunctions where, upon substitution $b \to a = x_0$, in

(53) the integration bounds are exchanged and in (57) the phase shift is $-\pi/4$ [5]. Of course the roles of the classically allowed and forbidden regions interchange too.

3.4 Born-Sommerfeld rule

Having computed the bound states of a binding potential, we want to compute their eigenenergies. Refer again to the situation in figure 5 with exactly two turning points: since the observable $|\psi(x)|^2$ must be the same whether we apply the connection rules at a or b, then equating the two versions of (57) and lifing the cosinuses leads to [5]

$$\int_a^x \frac{p(y)}{\hbar}\mathrm{d}y - \frac{\pi}{4} = \int_b^x \frac{p(y)}{\hbar}\mathrm{d}y + \frac{\pi}{4} + n\pi \qquad (58)$$

for some $n \in \mathbb{N}$, which can be reshuffled into the **Born-Sommerfeld quantization rule** [5]

$$\int_a^b p(x)\mathrm{d}x = \pi\hbar\left(n + \frac{1}{2}\right). \qquad (59)$$

The criterion (49) takes the form $n \gg 1$ because the rule behaves as $O(L/\lambda)$, nevertheless it sometimes gives exact results even for natural n [5], such as in the case of the harmonic oscillator of potential $V(x) = m\omega^2x^2/2$ and turning points $b = -a = \sqrt{2E/m\omega^2}$: the integration is the area of a semicircle and solving for E leads to the expected result $E = \hbar\omega(n + 1/2)$.

4 Conclusions

Feynman's path integral method was derived, its equivalence with the Schrödinger's equation was explicitated, the technique of separable Lagrangians was shown, the path integral was applied to statistical physics through a Wick rotation that was formally justified and the typical examples of the free particle and the harmonic oscillator were tackled. The method was proven to be extremely powerful since it bypasses the complicated resolution of the time-dependent Schrödinger's equation.

The WKB approximation was described, its range of validity was discussed, connection rules for the WKB wavefunctions were obtained and they were applied to compute bound states and to derive the Born-Sommerfeld rule. Albeit it remains an approximation, we saw that for specific systems it can lead to exact results.

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A Gaussian integral

For any $a, b, c \in \mathbb{C}$ with $\mathrm{Re}(a) > 0$ it is

$$\int \mathrm{d}x\, e^{-ax^2+bx+c} = \sqrt{\frac{\pi}{a}}\exp\left(\frac{b^2}{4a} + c\right). \qquad (60)$$

B Complex integration

For any $f(z) \in C^0(D)$ with $D \subset \mathbb{C}$ and for any regular path $C \subset D$ parametrized by $z(\lambda)$ with $\lambda \in [a; b] \subset \mathbb{R}$ and $a < b$ it is defined

$$\int_C \mathrm{d}z\, f(z) = \int_a^b \mathrm{d}\lambda\, \dot{z}(\lambda) f(z(\lambda)). \qquad (61)$$

C Trigonometric properties

For any $x \in \mathbb{R}$ it is

$$\begin{cases} \sin(ix) = i\sinh(x) \\ \cos(ix) = \cosh(x) \end{cases} \qquad (62)$$