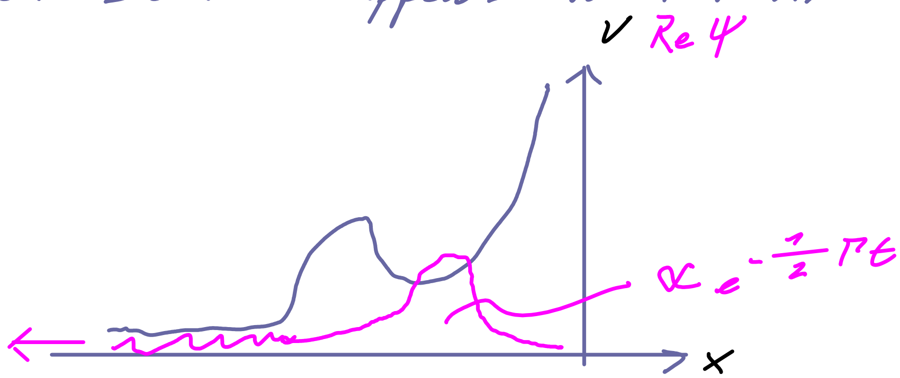
2 Tunneling rate from the WKB approximation to the Schrödinger equation

Eventually, we are interested in functional techniques for calculating tunneling rates. Here, for comparison, we discuss tunneling in the canonically quantized theory. We go beyond the leading WKB approximation what leads to the picture of a state that exponentially decays through a tunneling current.

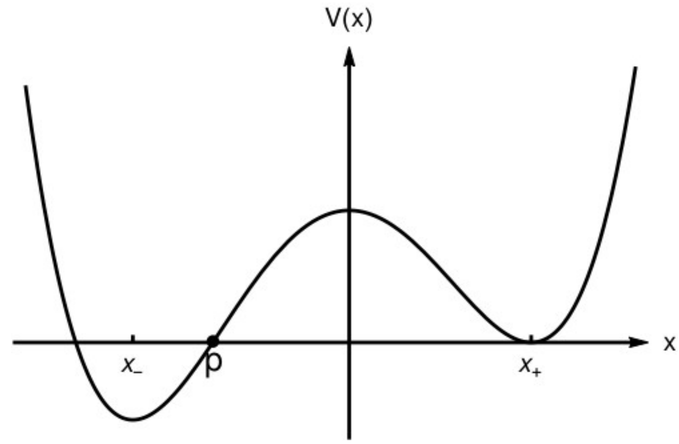
In particular, we will show that the canonically quantized solution appeals to intuition:



There is a "false ground state" that decays exponentially in time, a WKB piece penetrating the barrier and finally a probability flux escaping from that whole setup.

This picture is very clear & immediately plausible in comparison to the Euclidean/functional construction. Perhaps it is not in (many?) textbooks because of the cumbersome calculation. One of our aims is to compare the Schrödinger and functional approach and match the different parts of the calculations.

Particle trapped in false ground state (only makes approximate sense) escapes on classically forbidden path through the barrier toward global minimum x_- (where true ground state is located)



Here: Complete leading order expression for the decay rate using basic methods of quantum mechanics (QM):

1. WKB approximation inside the barrier
2. Construct approximate false ground state
3. Match 1 & 2
4. Approximate wave function for $x<p$ by an escaping wave
5. Decay rate as imaginary part of energy eigenvalue
6. Consistency check: Decay rate from probability flux

Parametrization of the problem: (QFT-like units)

$$L = \frac{1}{2}\dot{x}^2 - V(x)$$

$$H = \frac{1}{2}\dot{x}^2 + V(x) = \frac{1}{2}p^2 + V(x)$$

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

① Around x_+: $\quad V(x) \simeq \frac{1}{2}m^2(x_+ - x)^2$

(NB m^2 has here the meaning of a spring constant — recall for harmonic oscillator
$V = \frac{1}{2}kx^2 = \frac{1}{2}m\omega^2x^2$)

Zero-point energy of false ground state:

$$E = \hbar m\left(\frac{1}{2} + \varepsilon\right)$$

where ε is a small correction

Define $\quad \varkappa(x) = \sqrt{2(V(x) - E)}$

⟶ The leading order WKB solution for $V(x) \gg E$ and to zeroth order in ε is of the form:

$$\psi_{WKB}(x) = \frac{c_1}{\sqrt{\varkappa(x)}}\, e^{\frac{1}{\hbar}\int_{x_p}^{x} dx'\,\varkappa(x')} + \frac{c_2}{\sqrt{\varkappa(x)}}\, e^{-\frac{1}{\hbar}\int_{x_p}^{x} dx'\,\varkappa(x')}$$

To determine suitable approximations to the integrals, it is useful to consider solutions to the equations of motion in the upside-down potential with particular boundary conditions on the motion:

$\overline{x}(\tau=0)=x_p$

$\dot{\overline{x}}(\tau=0)=0$

$$\Longrightarrow \quad \frac{d\overline{x}(\tau)}{d\tau}=\sqrt{2\,V(\overline{x}(\tau))}$$

$$\Longrightarrow \quad \tau=\int_{x_p}^{x} dx' \frac{1}{\sqrt{2V(x')}}$$

For $\tau \to \infty$, $\overline{x}(\tau)$ approaches x_+ exponentially slow:

$$\frac{d\overline{x}(\tau)}{d\tau} \approx m\,(x_+ - \overline{x}(\tau)) \Longrightarrow \frac{d\overline{x}(\tau)}{d\tau} \approx \sqrt{B}\,\frac{A}{\sqrt{m}}\,e^{-m\tau}$$

We introduce here two normalization factors for convenience further down the road.

Equating these two expressions and solving for τ:

$$\tau=-\frac{1}{m}\log\left(\frac{m^{\frac{3}{2}}}{A\sqrt{B}}(x_+-\overline{x})\right)+\mathcal{O}(x_+-\overline{x})$$

$$=\int_{x_p}^{\overline{x}} dx' \frac{1}{\sqrt{2V(x')}}$$

Note: $V(x) \gg E \iff (x_+ - x)^2 \gg \frac{\hbar}{m}$

$\longrightarrow$ In this region, expand

$$\varkappa(x) \simeq \sqrt{2V(x)}\left(1 - \frac{E}{2V(x)}\right)$$

In case it holds in addition that $V(x) \simeq \frac{1}{2} m^2 (x_+ - x)^2$ we can approximate $\varkappa(x) \simeq m(x_+ - x)$.

$\longrightarrow$ For the integrals in the exponents of the WKB ansatz, we may write:

$$\int_{x_p}^{x} dx' \sqrt{2V(x')} = \int_{x_p}^{x_+} dx' \sqrt{2V(x')} + \int_{x_+}^{x} dx' \sqrt{2V(x')}$$

$$\simeq \frac{B}{2} + \int_{x_+}^{x} dx' \sqrt{m^2 (x_+ - x')^2}$$

$$= \frac{B}{2} - \frac{1}{2} m (x_+ - x)^2$$

Note that $\frac{B}{2}$ is the action for the motion in the upside-down potential:

$$\frac{B}{2} = \int_0^\infty d\tau \left(\frac{1}{2}\dot{\bar{x}}^2(\tau) + V(\bar{x}(\tau))\right) = \int_0^\infty d\tau\, \dot{\bar{x}}^2(\tau) = \int_0^\infty d\tau \frac{d\bar{x}(\tau)}{d\tau} \sqrt{2V(\bar{x}(\tau))}$$

$$= \int_{x_p}^{x_+} dx' \sqrt{2V(x')}$$

Recall:

$$\int_{x_p}^{x} dx' \frac{1}{\sqrt{2V(x)}} = -\frac{1}{m} \log\left(\frac{m^{\frac{3}{2}}}{A\sqrt{B}} (x_+ - x)\right)$$

Plugging all this back into the WKB ansatz, we find:

$$\psi_{WKB}(x) = \frac{c_1}{\sqrt{m(x_+-x)}} \exp\left\{\frac{1}{\hbar}\left(\frac{B}{2} - \frac{m}{2}(x_+-x)^2 + \frac{E}{m}\log\left(\frac{m^{\frac{3}{2}}}{\sqrt{B}A}(x_+-x)\right)\right)\right\}$$

$$+ \frac{c_2}{\sqrt{m(x_+-x)}} \exp\left\{-\frac{1}{\hbar}\left(\frac{B}{2} - \frac{m}{2}(x_+-x)^2 + \frac{E}{m}\log\left(\frac{m^{\frac{3}{2}}}{\sqrt{B}A}(x_+-x)\right)\right)\right\}$$

And with $E = \hbar m\left(\frac{1}{2}+\varepsilon\right)$:

$$\psi_{WKB}(x) = \left\{c_1\, e^{\frac{B}{2\hbar}} B^{-\frac{1}{4}} A^{-\frac{1}{2}} m^{\frac{1}{4}} e^{-\frac{m}{2\hbar}(x_+-x)^2}\right.$$
$$\left. + c_2\, e^{-\frac{B}{2\hbar}} B^{\frac{1}{4}} A^{\frac{1}{2}} m^{-\frac{5}{4}} \frac{1}{x_+-x} e^{\frac{m}{2\hbar}(x_+-x)^2}\right\} * (1+\Theta(\varepsilon))$$

As a function of x, these solutions are valid in the region where the quadratic approximation is and at the same time $E \ll V$. When ignoring to this end the solution $\propto c_1$, we have found the familiar result that the tunneling rate is $\Gamma \sim |\psi|^2 \sim e^{-\frac{B}{\hbar}}$

To make a first estimate, we can use that in the false ground state ($x_0 = \sqrt{\frac{\hbar}{\omega m}} \longrightarrow \sqrt{\frac{\hbar}{m}}$)

$$\langle p^2 \rangle = \langle \dot{x}^2 \rangle = \frac{1}{2}\frac{\hbar^2}{x_0^2} = \frac{1}{2}\hbar m$$
$$\langle x^2 \rangle = \frac{x_0^2}{2} = \frac{1}{2}\frac{\hbar}{m}$$

$\longrightarrow$ Rate for hitting the barrier

$$\Gamma_{barrier} \sim \sqrt{\frac{\langle p^2 \rangle}{\langle x^2 \rangle}} = m$$

Multiply with amplitude of the wave function

$\longrightarrow$

$$\Gamma \sim m|\psi|^2 = m\, e^{-\frac{B}{\hbar}}$$

This is a familiar estimate. We can do better however by constructing the full solution by matching to the regions where the form of ψ_{WKB} is not valid. One can apply the standard procedure that makes use of Airy functions.

② False ground state solution

Around $x = x_+$, we have the Schrödinger equation

$$-\frac{\hbar^2}{2}\partial_x^2\psi(x) + \frac{1}{2}m^2(x-x_+)^2\psi(x) = E\,\psi(x)$$

Treat ε as a perturbation.

For $\varepsilon = 0$, we find the solutions

$$\psi_1(x) = m^{\frac{1}{4}}\, e^{-\frac{m}{2\hbar}(x_+-x)^2}$$

$$\psi_2(x) = \frac{1}{m^{\frac{1}{4}}(x_+-x)}\, e^{\frac{m}{2\hbar}(x_+-x)^2}$$

In particular,

$$\frac{-\frac{\hbar^2}{2}\partial_x^2\psi_2(x) + \frac{1}{2}m^2(x-x_+)^2\psi_2(x)}{\psi_2(x)} = \frac{1}{2}\hbar m - \frac{\hbar^2}{(x-x_+)^2}$$

i.e. $\psi_2(x)$ is valid for $(x-x_+)^2 \gg \frac{\hbar}{m}$

Wronskian:

$$\psi_1(x)\,\partial_x \psi_2(x) - \psi_2(x)\,\partial_x \psi_1(x) = -\frac{2m}{\hbar} + \mathcal{O}\left(\frac{1}{(x-x_+)^2}\right)$$

Now for $\varepsilon \neq 0$, use perturbation theory:

$$\psi(x) = \psi_1(x) + \delta\psi(x)$$

$\longrightarrow$

$$-\frac{\hbar^2}{2}\partial_x^2\,\delta\psi(x) + \frac{1}{2}m^2(x-x_+)^2\,\delta\psi(x) = \hbar m\,\varepsilon\,\psi_1(x)$$

Now make use of the following:

Let $\{u_1, u_2\}$ be two solutions to the homogeneous equation pertaining to

$$u''(x) + p(x)\,u'(x) + q(x)\,u(x) = f(x)$$

Then a particular solution is given by

$$u(x) = -u_2(x)\int_x^\infty dx'\,\frac{u_1(x')\,f(x')}{W[u_1(x'), u_2(x')]} + u_1(x)\int_x^\infty dx'\,\frac{u_2(x')\,f(x')}{W[u_1(x'), u_2(x')]}$$

$2u_2'u_1 f + u_2 u_1' f$
$-2u_1' u_2 f - u_1 u_2' f$
$= u_1 u_2' f - u_2 u_1' f$

where W is the Wronskian

To apply this, we rewrite the equation for $\delta\varphi$ as

$$\partial_x^2\,\delta\psi(x) - \frac{m^2}{\hbar^2}(x-x_+)^2\,\delta\psi(x) = -2\frac{m}{\hbar}\,\varepsilon\,\psi_1(x)$$

and identify

$$f(x) = -2\frac{m}{\hbar}\,\varepsilon\,\psi_1(x)$$

$\Longrightarrow$

$$\delta\psi(x) = -\frac{\hbar}{2m}\left(-\frac{2\varepsilon m}{\hbar}\right)\int_x^\infty dx' \left\{-\psi_2(x)\psi_1^2(x') + \psi_1(x)\psi_1(x')\psi_2(x')\right\}$$

$$= -\varepsilon\sqrt{\pi\hbar}\,\psi_2(x) = -\varepsilon\frac{\sqrt{\pi\hbar}}{m^{\frac{1}{4}}(x_+-x)}\, e^{\frac{m}{2\hbar}(x_+-x_-)^2}$$

The upshot is that by using ε as a perturbation to the Gaussian approximation to the false ground state equation & solution, we obtain

$$\psi(x) = N\left\{ m^{\frac{1}{4}} e^{-\frac{m}{2\hbar}(x_+-x)^2}(1+\mathcal{O}(\varepsilon)) - \frac{\varepsilon\sqrt{\pi\hbar}}{m^{\frac{1}{4}}(x_+-x)}\, e^{\frac{m}{2\hbar}(x_+-x)^2}\right\}$$

with some normalization N.

This form is valid for $(x-x_+)^2 \gg \frac{\hbar}{m}$ and can be matched to the WKB approximation in the region where the quadratic approximation remains valid.

③ Now we match the false ground state solution to the WKB approximation. This way, we can write $\frac{c_1}{c_2}$ as a function of A, B, m and ε.

The approximations given by the WKB solution as well as the false ground state are valid for $(x-x_+) \gg \frac{\hbar}{m}$. Given their form, we can match these without further ado:

$$\frac{c_1}{c_2} e^{\frac{B}{\hbar}} B^{-\frac{1}{2}} A^{-1} m^{\frac{3}{2}} = -m^{\frac{1}{2}} \frac{1}{\varepsilon\sqrt{\pi\hbar}} \iff$$

$$m\varepsilon = -\frac{c_2}{c_1}\sqrt{\frac{B}{\pi\hbar}}\, A\, e^{-\frac{B}{\hbar}}$$

④ For $x < x_p$, the solution should go to an outgoing wave. The transition region can be treated approximately using the Airy equation. To obtain it, define

$$y = x - x_p = \left(\frac{\hbar^2}{2V'(x_p)}\right)^{\frac{1}{3}} z$$

$$\left(-\frac{\hbar^2}{2}\frac{\partial^2}{\partial x^2} + V(x)\right)\psi(x) = E\,\psi(x)$$

$\longrightarrow$

$$\left(-\frac{\hbar^2}{2}\frac{\partial^2}{\partial x^2} + V'(x_p)(x-x_p)\right)\psi(x) = 0$$

$\longrightarrow$

$$\left(-\frac{\hbar^2}{2}\left(\frac{2V'(x_p)}{\hbar^2}\right)^{\frac{2}{3}}\frac{\partial^2}{\partial z^2} + 2^{-\frac{1}{3}}\left(\hbar V'(x_p)\right)^{\frac{2}{3}} z\right)\psi(z) = 0$$

$\longrightarrow$

$$\partial^2\psi(z) - z\psi(z) = 0$$

The solutions are $Ai(z)$ and $Bi(z)$ with the asymptotics

$$\left.\begin{aligned} Ai(z) &\simeq \frac{1}{2\sqrt{\pi}} z^{-\frac{1}{4}} e^{-\frac{2}{3}z^{\frac{3}{2}}} \\ Bi(z) &\simeq \frac{1}{\sqrt{\pi}} z^{-\frac{1}{4}} e^{\frac{2}{3}z^{\frac{3}{2}}} \end{aligned}\right\} \text{ for } z \to \infty$$

$$\left.\begin{aligned} Ai(z) &\simeq \frac{1}{\sqrt{\pi}} |z|^{-\frac{1}{4}} \sin\left(\frac{2}{3}|z|^{\frac{3}{2}} + \frac{\pi}{4}\right) \\ Bi(z) &\simeq \frac{1}{\sqrt{\pi}} |z|^{-\frac{1}{4}} \cos\left(\frac{2}{3}|z|^{\frac{3}{2}} + \frac{\pi}{4}\right) \end{aligned}\right\} \text{ for } z \to -\infty$$

Compare this with the WKB solution for $x \gtrsim x_p$:

$$\psi_{WKB}(x) = \frac{c_1}{\sqrt{\varkappa(x)}} e^{\frac{1}{\hbar}\int_{x_p}^{x} dx'\, \varkappa(x')} + \frac{c_2}{\sqrt{\varkappa(x)}} e^{-\frac{1}{\hbar}\int_{x_p}^{x} dx'\, \varkappa(x')}$$

where

$$\varkappa(x) \approx \sqrt{2V(x)} \approx \sqrt{2V'(x_p)(x-x_p)} = \left(2\hbar V'(x_p)\right)^{\frac{1}{3}} \sqrt{z}$$

$$= \hbar \frac{dz}{dx} \sqrt{z}$$

From this, we see that for $x < x_p$, we have

$$\psi(x) = \frac{c_1}{\sqrt{|\varkappa(x)|}} \cos\left(\frac{1}{\hbar}\int_{x}^{x_p} dx'\, |\varkappa(x')| + \frac{\pi}{4}\right)$$

$$+ \frac{2c_2}{\sqrt{|\varkappa(x)|}} \sin\left(\frac{1}{\hbar}\int_{x}^{x_p} dx'\, |\varkappa(x')| + \frac{\pi}{4}\right)$$

Now we can fix the ratio of c_1 and c_2 by imposing a purely outgoing wave

$$\sim e^{-\frac{i}{\hbar}\left(\int_x^{x_p} dx' \, |\chi(x')| + \frac{\pi}{4}\right)}$$

$$\longrightarrow c_1 = 2i\, c_2$$

Substituting that into the matching condition of the false ground state with the WKB approximation yields

$$m\,\varepsilon = -\frac{c_2}{c_1}\sqrt{\frac{B}{\pi\hbar}}\, A\, e^{-\frac{B}{\hbar}} = \frac{i}{2}\sqrt{\frac{B}{\pi\hbar}}\; A\; e^{-\frac{B}{\hbar}}$$

(5) Since the amplitude $\sim e^{\frac{i}{\hbar}Et}$, the decay rate is

$$\Gamma = \frac{2}{\hbar}\,\mathrm{Im}\,E = \frac{2}{\hbar}\,\mathrm{Im}\left[\hbar\, m\,\varepsilon\right] = \sqrt{\frac{B}{\pi\hbar}}\, A\, e^{-\frac{B}{\hbar}}$$

We recall here that A enters through the solution for $\overline{x}(\tau)$

(6) We can also interpret the result in terms of probabilities and probability currents.
The probability of finding the particle at the false ground state is dominated by the Gaussian piece of the WKB approximation:

$$P = |c_1|^2\, e^{\frac{B}{\hbar}}\, B^{-\frac{1}{2}}\, A^{-1}\, m^{\frac{1}{2}} \int dx\, e^{-\frac{m}{\hbar}(x_f - x)^2}$$

$$= |c_1|^2\, e^{\frac{B}{\hbar}}\, B^{-\frac{1}{2}}\, A^{-1}\, \sqrt{\pi\hbar}$$

The flux into the region of the true ground state is:

$$j = \frac{\hbar}{2i}\left(\psi^* \partial_x \psi - \psi \partial_x \psi^*\right) = -|c_1|^2$$

This gives the decay rate

$$\Gamma = -\frac{j}{P} = e^{-\frac{B}{\hbar}} \sqrt{\frac{B}{\pi\hbar}}\, A$$

in agreement with the result from the imaginary part of the energy.