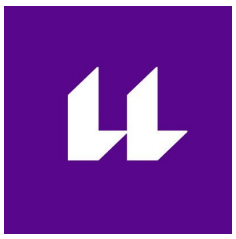

Universidad de La Laguna

Final degree project

The connection between classical and quantum mechanics: semi-classical models

Pablo Díaz Calzadilla

supervised by
Dr. José María Gómez Llorente

Contents

Abstract

Históricamente, los fenómenos y sistemas en la mecánica cuántica se comenzaron a estudiar mediante el establecimiento de analogías entre ellos y su homólogo clásico, siendo la mayoría de estos modelos iniciales, en realidad, modelos semiclásicos. Entre las propiedades mas destacables de dichos tratamientos semiclásicos esta la capacidad de dar cuenta, de forma relativamente simple e intuitiva, de fenómenos de difícil comprensión y alejados de la realidad clásica, revelando las conexiones entre el movimiento clásico de los sistemas físicos y sus comportamientos cuánticos. También es importante su utilidad para el análisis de la espectroscopía de sistemas complejos cuya dinámica clásica es caótica, como es el caso de las moléculas en estados de vibración excitados o el átomo de Hidrógeno en presencia de campos magnéticos de alta intensidad.

En lo referido al trabajo en particular, se estudiará la utilización del modelo WKB para la resolución de la ecuación de Schrödinger. Además mediante un ejemplo práctico, se investigará el tratamiento semiclásico del efecto túnel cuántico y la contribución de las trayectorias clásicas complejas a dicho fenómeno.

En concreto, el trabajo consta de dos partes bien diferenciadas. En la primera se llevará a cabo un desarrollo teórico en que se obtendrán las expresiones en dicha aproximación semiclásica de las funciones de onda en el caso estacionario, para una partícula en una dimension sometida a un cierto potencial, y no estacionario, para el caso de una partícula en el espacio tridimensional también sometida a un potencial suave, el propagador y la función de Green, y finalmente, la densidad de estados. Además en esta sección se obtendrán también las condiciones bajo las que esta aproximación es válida, así como la condición de cuantización de Bohr-Sommerfeld, antiguamente empleada en la obtención de la energías de los estados estacionarios. A continuación, pasamos a aplicar dicha idea al problema de una partícula en un potencial cúbico, cuyo espectro será continuo y presentará estados resonantes para el cual obtendremos acciones y periodos (tanto en el pozo como bajo la barrera) sumando las contribuciones de las posibles trayectorias clásicas (reales y complejas). Finalmente, a esta sección se añaden las representaciones gráficas de dichas magnitudes frente a la energía.

Part I
Theoretical background

En esta primera sección se dará un trasfondo teórico a los métodos semiclásicos, es decir, vamos a obtener la forma de diferentes operadores (propagador y función de Green) y funciones de onda (casos estacionario y no estacionario) en el límite semiclásico.

Nuestro primer paso consistirá en obtener la función de onda para una sola partícula en una dimensión el caso estacionario, haciendo uso de la ecuación de Scrödinger independiente del tiempo. Las aproximaciones aquí realizadas nos llevaran a conocer los límites en los que nuestro modelo dejará de ser aplicable y obtendremos por último la regla de cuantización de Bohr-Sommerfeld.

Después pasamos al caso no estacionario, haciendo uso de una forma para la función de onda similar al del caso anterior. Finalmente obtenemos el propagador y la función de Green. La parte imaginaria de la traza de esta última nos dará la densidad de estados.

1 WKB model

The WKB approximation is a method used in this case for a semi-classical calculation in quantum mechanics in which the wavefunction is recast as an exponential function, and its phase is taken to be slowly changing in time. WKB is an acronym for Wentzel-Kramer-Brillouin, the three physicists who developed it in 1926. In our case we are going to follow the theoretical development by *Landau* and *Lifshitz* [1] and *Cvitanovic* [2].

1.1 WKB ansatz

As in the case of wave optics, which is reduced to geometric optics when the wavelength tends to zero, if the De Brolie wavelengths of the particles were small compared to the condition of our problem, their properties look like those of a classical system. Analyzing the time-independent *Schrödinger equation*

$$\frac{\hbar^2}{2m}\triangle\psi + (E - V)\psi = 0$$

and substituting a solution like

$$\psi = \exp(\frac{i}{\hbar}\sigma), \tag{1}$$

we obtain

$$\frac{\hbar^2}{2m}\nabla(\nabla(e^{\frac{i}{\hbar}\sigma})) + (E - V)e^{\frac{i}{\hbar}\sigma} = 0.$$

Taking into account that

$$\nabla(e^{\frac{i}{\hbar}\sigma}) = \frac{\partial(e^{\frac{i}{\hbar}\sigma})}{\partial x}\hat{i} + \frac{\partial(e^{\frac{i}{\hbar}\sigma})}{\partial y}\hat{j} + \frac{\partial(e^{\frac{i}{\hbar}\sigma})}{\partial z}\hat{k} =$$

$$= \frac{\partial\sigma}{\partial x}[\frac{\partial(e^{\frac{i}{\hbar}\sigma})}{\partial\sigma}]\hat{i} \; + \; \frac{\partial\sigma}{\partial y}[\frac{\partial(e^{\frac{i}{\hbar}\sigma})}{\partial\sigma}]\hat{j} \; + \; \frac{\partial\sigma}{\partial z}[\frac{\partial(e^{\frac{i}{\hbar}\sigma})}{\partial\sigma}]\hat{k} \; = \nabla\sigma(\frac{\partial(e^{\frac{i}{\hbar}\sigma})}{\partial\sigma}) = \nabla\sigma(\frac{i}{\hbar}e^{\frac{i}{\hbar}\sigma})$$

and with the property, $\nabla(\mathbf{A}\cdot\mathbf{B}) = \mathbf{A}(\nabla\mathbf{B}) + \mathbf{B}(\nabla\mathbf{A})$, which leads us to

$$\nabla[\nabla\sigma(\frac{i}{\hbar}e^{\frac{i}{\hbar}\sigma})] = \frac{i}{\hbar}(\triangle\sigma)e^{\frac{i}{\hbar}\sigma} - \frac{1}{\hbar^2}(\nabla\sigma)^2 e^{\frac{i}{\hbar}\sigma}$$

we finally find the equality

$$\frac{1}{2m}(\nabla\sigma)^2 - \frac{i\hbar}{2m}\triangle\sigma = E - V \tag{2}$$

By its properties the system is considered semi-classical, so σ could be expanded in powers of the "small" $\hbar$ parameter

$$\sigma = \sigma_0 + \frac{\hbar}{i}\sigma_1 + (\frac{\hbar}{i})^2\sigma_2 + ... \tag{3}$$

In the most simple case, the one-dimensional motion of a particle, equation (2) is reduced to

$$\frac{1}{2m}(\frac{d\sigma}{dx})^2 - \frac{i\hbar}{2m}\frac{d^2\sigma}{dx^2} = E - V(x). \tag{4}$$

By substituting equation (3) in equation (4), the lowest order approximation σ=σ_0, is a solution of the equation.

$$\frac{1}{2m}(\frac{d\sigma_0}{dx})^2 = E - V(x), \;\; \text{i.e.,}$$

$$\sigma_0 = \int dx\, p(x),$$

where $p(x) = \pm\sqrt{2m(E - V(x))}$, is the classical momentum.

We only could neglect $\hbar$ term in equation (4) if it is small in comparison with the other one. In other words,

$$\hbar|\sigma^{''}/(\sigma^{'})^2| = |d(\hbar/\sigma^{'})/dx| \ll 1.$$

In first order approximation $\sigma^{'} = \pm p$ and we have

$$|d(\lambda/2\pi)/dx| \ll 1,$$

where $\lambda(x) = \dfrac{2\pi\hbar}{p(x)}$ is the x-dependent de Broglie wave-length. Here, we have obtained a quantitative condition for the validity of the semi-classical approach. Also, taking into account that

$$\frac{dp}{dx} = -\frac{m}{p}\frac{dV}{dx} = \frac{m|F|}{p},$$

we find the condition

$$\frac{m\hbar|F|}{p^3} \ll 1,$$

where $F = -dV/dx$ is the classical force. From here it follows that close to the *turning points* ($p(x) = 0, E = V(x)$), where classically the particle stops and starts to move in the opposite way, the semi-classical approximation fails.

Regarding the next term in (3), the first order terms in $\hbar$ leads us to

$$\frac{d\sigma_0}{dx}\frac{d\sigma_1}{dx} + \frac{1}{2}\frac{d^2\sigma_0}{dx^2} = 0$$

As $\sigma_0' = p$, we finally obtain

$$\sigma_1' = \frac{d\sigma_1}{dx} = -\frac{1}{2}\frac{\sigma_0''}{\sigma_0'} = -\frac{1}{2}\frac{p'}{p} \quad \text{therefore} \quad \sigma_1 = -\frac{1}{2}\ln p(x) + C.$$

Now we have an expression for σ_0 and σ_1 so we obtain a semi-classical wavefunction (1) with the form

$$\psi = \frac{C_1}{\sqrt{p}} e^{\frac{i}{\hbar}\int p dx} + \frac{C_2}{\sqrt{p}} e^{-\frac{i}{\hbar}\int p dx} = \frac{C_1}{\sqrt{p}} e^{\frac{i}{\hbar}S} + \frac{C_2}{\sqrt{p}} e^{-\frac{i}{\hbar}S}. \tag{5}$$

In this expression, the presence of the factor $1/\sqrt{p}$ means that the probability of finding the particle between x and $x + dx$, $|\psi|^2$, is proportional to $1/p$. That is exactly what is expected for a *semi-classical particle*, which spends a time in the interval between x and $x + dx$ inversely proportional to its momentum.

1.2 Bohr-Sommerfield quantization condition

If $x = a$ is a *turning point* ($V(a) = E, p(a) = 0$), and if for $x > a$, $V > E$, then the classical momentum is imaginary and the region is classically banned. Because of this, the quantum wavefunction has to tend to zero in this region, which leads us to

$$\psi = \frac{C}{2\sqrt{|p|}} \exp(-\frac{1}{\hbar}|\int_a^x p\, dx|) \quad ;\ x > a. \tag{6}$$

This expression corresponds, in fact, to the second term in (5).

On the other hand, on the classically allowed region, the wavefunction is the linear combination of the two semi-classical solutions of the Schrödinger equation

$$\psi = \frac{C_1}{\sqrt{p}} \exp(\frac{i}{\hbar}\int_a^x p\, dx) + \frac{C_2}{\sqrt{p}} \exp(-\frac{i}{\hbar}\int_a^x p\, dx) \quad ;\ x < a. \tag{7}$$

In order to obtain the value of C, C_1 and C_2,it would be necessary to follow the wavefunction across $x = a$, where the semi-classical solution is not applicable. It is possible to avoid this problem considering ψ as a function of

a complex variable x, which cross from negative to positive values of $x-a$ sufficiently far from $x=a$, where the semi-classical condition is always met.

First, the wavefunction will surround the point $x=a$ from right to left in a semi-circumference with big radio in the upper complex half-plane of x. While we go through this contour, the function (6) should be transformed in the second term of (7), due to the fact that the first one tends to zero exponentially. As in this process the phase of the difference $V(x)-E$ increases in π, we obtain $C_2 = \frac{1}{2}Ce^{-i\pi/4}$. In the same way when we travel through the semi-circumference in the lower half-plane, (6) turns into the first term of (7) with the coefficient $C_1 = \frac{1}{2}Ce^{i\pi/4}$. This leads us finally to

$$\psi = \frac{C}{2\sqrt{|p|}} \exp(-\frac{1}{\hbar}|\int_a^x p\,dx|) \quad ;\ x > a.$$

$$\psi = \frac{C}{\sqrt{p}} \cos(\frac{1}{\hbar}\int_a^x p\,dx + \frac{\pi}{4}) = \frac{C}{\sqrt{p}} \sin(\frac{1}{\hbar}\int_x^a p\,dx + \frac{\pi}{4}) \quad ;\ x < a.$$

With this result we could deduce the condition which determines the quantum energy levels in the semi-classical case. If we take into account the one-dimensional movement of one particle in a potential well, the classical domain, $a \leq x \leq b$, is restricted by the turning points. The wavefunction for $x > a$ is

$$\psi = \frac{C}{\sqrt{p}} \sin(\frac{1}{\hbar}\int_a^x p\,dx + \frac{\pi}{4}).$$

The wavefunction for $x < b$ is

$$\psi = \frac{C'}{\sqrt{p}} \sin(\frac{1}{\hbar}\int_x^b p\,dx + \frac{\pi}{4}).$$

Necessarily this expressions have to coincide in all the interval $a \leq x \leq b$, so the sum of the phases have to be a whole multiple of π,

$$\frac{1}{\hbar}\int_a^b p\,dx + \frac{\pi}{2} = (n+1)\pi$$

$$\oint p\,dx = 2\pi\hbar(n+\frac{1}{2}) \tag{8}$$

with $C = (-1)^n C'$ and $\oint p\,dx = 2\int_a^b p\,dx$. This condition determines the stationary states of a particle in the semi-classical approximation and it is known as the Bohr-Sommerfeld quantification rule of the semi-classical quantum theory.

Besides, in order to normalize the wavefunction, we integrate $|\psi|^2$ between $x=a$ and $x=b$

$$\int |\psi|^2\,dx \cong \frac{C^2}{2}\int_a^b \frac{dx}{p(x)} = \frac{\pi C^2}{2m\omega} = 1,$$

where we have substituted the sine square by its middle value 1/2 and taking into account that $\omega = 2\pi/T$, which is a function of the energy, the semi-classical wavefunction is

$$= \sqrt{\frac{2m\omega}{p\pi}} \sin(\frac{1}{\hbar}\int_x^b p\, dx + \frac{\pi}{4}).$$

2 Semi-classical evolution

In the last section, we have been working with the stationary states of a 1D particle moving in a smooth potential. Now, we are going to work with the non stationary solutions corresponding to a particle in a d-dimensional space, with mass m and coordinates $\mathbf{q} = (q_1, q_2, ..., q_d)$, moving in an external potential $V(\mathbf{q})$. The particle wavefunction $\psi(\mathbf{q}, t)$ is a solution of the time dependent Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\psi(\mathbf{q},t) - \frac{\hbar^2}{2m}[\sum_{i=1}^{d}\frac{\partial^2}{\partial q_i^2}\psi(\mathbf{q},t)] - V(\mathbf{q})\psi(\mathbf{q},t) = 0.$$

Taking into account the last section wavefunction our ansatz will be

$$\psi(\mathbf{q},t) = A(\mathbf{q},t)e^{\frac{i}{\hbar}R(\mathbf{q},t)},$$

with rapidly varying phase $R(\mathbf{q}, t)$ and and slowly varying amplitude $A(\mathbf{q}, t)$, both real magnitudes.

If $A \neq 0$ and we separate the real and imaginary part, we get two equations, the real part governs the time evolution of the phase

$$\frac{\partial R}{\partial t} + \frac{1}{2m}(\sum_{i=1}^{d}\frac{\partial R}{\partial q_i})^2 + V(q) - \frac{\hbar^2}{2mA}\sum_{i=1}^{d}\frac{\partial^2 A}{\partial q_i^2} = 0, \tag{9}$$

and the imaginary part the time evolution of amplitude

$$\frac{\partial A}{\partial t} + \frac{1}{m}\sum_{i=1}^{d}\frac{\partial A}{\partial q_i}\frac{\partial R}{\partial q_i} + \frac{A}{2m}\sum_{i=1}^{d}\frac{\partial^2 R}{\partial q_i^2} = 0. \tag{10}$$

Is important to see that the coupling term in (9) is of order $\hbar^2$ and thus small in the semi-classical limit $\hbar \longrightarrow 0$. Taking this into account equation (9) is finally the classical *Hamilton-Jacobi equation*,

$$\frac{\partial R}{\partial t} + H(\mathbf{q}, \mathbf{p}) = 0, \tag{11}$$

being $\mathbf{p} = \dfrac{\partial R}{\partial \mathbf{q}}$ the canonical momenta.

2.1 Hamilton's equations

In order to obtain the phase $R(\mathbf{q},t)$, and knowing that

$$\frac{dR}{dt} = \frac{\partial R}{\partial t} + \sum_{i=1}^{d} \frac{\partial R}{\partial q_i}\dot{q}_i = -H(\mathbf{p}(t),\mathbf{q}(t)) + \mathbf{p}(t)\dot{\mathbf{q}}(t), \tag{12}$$

we have to integrate equation (12), which leads us to

$$R(\mathbf{q},t) = R(\mathbf{q}',t_0) + R(\mathbf{q},t;\mathbf{q}',t_0)$$

$$R(\mathbf{q},t;\mathbf{q}',t_0) = \int_{t_0}^{t} d\tau[\dot{\mathbf{q}}(\tau)\mathbf{p}(\tau) - H(\mathbf{q}(\tau),\mathbf{p}(\tau))], \tag{13}$$

Our trajectory should satisfy a two-time boundary condition. At the final time (t), $\mathbf{q}(t) = \mathbf{q}$ and $\mathbf{p}(t)$ is arbitrary and, at the initial time (t_0), $\mathbf{q}(t_0) = \mathbf{q}'$ and $\mathbf{p}(t_0) = \mathbf{p}'$, which fulfills the relationship

$$\mathbf{p}' = \frac{\partial R}{\partial \mathbf{q}}(\mathbf{q}',t_0).$$

If energy is conserved the only time dependence of $H(\mathbf{q},\mathbf{p})$ is through $(\mathbf{q}(\tau),\mathbf{p}(\tau))$, so $R(\mathbf{q},t;\mathbf{q}',t_0)$ does not depend on t_0, but only on the elapsed time $t - t_0$. If we set $t_0 = 0$ we finally obtain

$$R(\mathbf{q},t) = R(\mathbf{q}',0) + R(\mathbf{q},\mathbf{q}',t).$$

When the energy is conserved, $H(\mathbf{q},\mathbf{p}) = E$, the $\int H(\mathbf{q},\mathbf{p})d\tau$ integral in (13) is Et. The other part is the *action*

$$S(\mathbf{q},\mathbf{q}',E) = \int_0^t d\tau\, \dot{\mathbf{q}}(\tau)\mathbf{p}(\tau) = \int_{\mathbf{q}'}^{\mathbf{q}} d\mathbf{q}\,\mathbf{p}. \tag{14}$$

By (13) we can say that the action is the Legendre transform of Hamilton's principal function

$$S(\mathbf{q},\mathbf{q}',E) = R(\mathbf{q},\mathbf{q}',t) + Et. \tag{15}$$

2.2 Semi-classical wavefuntion

In order to obtain the full solution of the Schrödinger equation, we have to integrate (10) too. To the leading order in $\hbar$, the gradient of R might be interpreted as the semi-classical momentum density

$$^*(\mathbf{q},t)(-i\hbar\sum_{i=1}^{d}\frac{\partial}{\partial q_i})\psi(\mathbf{q},t) = -i\hbar A\sum_{i=1}^{d}\frac{\partial A}{\partial q_i} + \rho\sum_{i=1}^{d}\frac{\partial R}{\partial q_i},$$

where $\rho(\mathbf{q},t) = A^2 = \psi^*\psi$. The equation (10) leads us the continuity equation,

$$\frac{\partial \rho}{\partial t} + \sum_{i=1}^{d}\frac{\partial}{\partial q_i}(\rho\nu_i) = 0.$$

Here, $\nu_i(\mathbf{q},t) = \dot{q}_i = \dfrac{p_i}{m}$ denotes the component i of a velocity field,

$$\nu_i(\mathbf{q},t) = \frac{1}{m}\frac{\partial}{\partial q_i}R(\mathbf{q},t).$$

In a small configuration space volume d^dq around a point $\mathbf{q}$ at time t, the number of particles in it is $\rho(\mathbf{q},t)d^dq$. Initially, this swarm of particles, are in a small volume d^dq' around $\mathbf{q}'$. The conservation of the particle number implies that

$$\rho(\mathbf{q}(t),t)d^dq = \rho(\mathbf{q}',0)d^dq',$$

so we finally obtain,

$$\rho(\mathbf{q}(t),t) = |\det\frac{\partial\mathbf{q}'}{\partial\mathbf{q}}|\rho(\mathbf{q}',0),$$

where the determinant is the Jacobian of the transformation $\mathbf{q} = \mathbf{q}(\mathbf{q}',t)$.

With these considerations, the semi-classical wavefunction at time t is

$$\psi_{sc}(\mathbf{q},t) = A(\mathbf{q},t)e^{\frac{i}{\hbar}R(\mathbf{q},t)} = \sqrt{\det\frac{\partial\mathbf{q}'}{\partial\mathbf{q}}}A(\mathbf{q'},0)e^{\frac{i}{\hbar}(R(\mathbf{q}',0)+R(\mathbf{q},\mathbf{q}',t))} =$$

$$= \sqrt{\det\frac{\partial\mathbf{q}'}{\partial\mathbf{q}}}e^{\frac{i}{\hbar}R(\mathbf{q},\mathbf{q}',t)}\psi(\mathbf{q}',0).$$

In this case we are considering that our initial wave function can be written in terms of single-valued functions $A(\mathbf{q}',0)$ and $R(\mathbf{q}',0)$. Besides, for short times, $R(\mathbf{q},t)$ will remain single-valued.

As time goes by, $\partial_{\mathbf{q}}R(\mathbf{q},t)$ can develop folds and consequently, the value of the phase is not unique, i.e., more than one trajectory will connect $\mathbf{q}'$ and $\mathbf{q}$ with different phases $R(\mathbf{q},\mathbf{q}',t)$ accumulated along these paths.

We expect different trajectories from $\mathbf{q}'$ to $\mathbf{q}$ which we will index by j and with different phases $R_j(\mathbf{q},\mathbf{q}',t)$.

Whenever the Lagrangian manifold develops a fold, the orientation of the pieces of the Lagrangian manifold changes $(\mathbf{q}, \frac{\partial R(\mathbf{q},t)}{\partial\mathbf{q}})$ with regard to the initial one, so the eigenvalues' sign changes at each fold crossing. So, to keep track of the signs we write the Jacobian determinant as

$$\det\frac{\partial\mathbf{q}'}{\partial\mathbf{q}}|_j = e^{-i\pi m_j(\mathbf{q},\mathbf{q}',t)}|\det\frac{\partial\mathbf{q}'}{\partial\mathbf{q}}|_j,$$

where the topological index of the trajectory, $m_j(\mathbf{q},\mathbf{q}',t)$, counts the number of sign changes of the Jacobian determinant on the way from $\mathbf{q}$ to $\mathbf{q}'$ along the $j-th$ trajectory.

Finally, the semi-classical aproximation to the wave function is a sum over possible trajectories that start at $\mathbf{q}'$ and end in $\mathbf{q}$ at time t, with each contribution weighted by the corresponding phase increment, the topological index and density,

$$\psi_{sc}(\mathbf{q},t) = \sum_j |\det\frac{\partial\mathbf{q}'}{\partial\mathbf{q}}|_j^{1/2}\ e^{\frac{i}{\hbar}(R_j(\mathbf{q},\mathbf{q}',t)-\frac{\pi}{2}\hbar m_j(\mathbf{q},\mathbf{q}',t))}\psi(\mathbf{q}_j',0). \qquad (16)$$

3 Semi-classical propagator

The *quantum evolution operator*, or the *propagator*, in the coordinate representation, satisfies the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}K(\mathbf{q},\mathbf{q}',t) = H(\mathbf{q},\mathbf{p})K(\mathbf{q},\mathbf{q}',t).$$

In terms of the stationary solutions, the non-stationary solutions of the time-dependent Scrödinger equation for time-independent Hamiltonian operators have the form

$$\psi(\mathbf{q},t) = \sum_n c_n e^{-iE_n t/\hbar}\phi_n(\mathbf{q}),$$

where the expansion coefficient c_n is given by

$$c_n = \int d\mathbf{q}\phi_n^*(\mathbf{q})\psi(\mathbf{q},0).$$

so we obtain

$$\psi(\mathbf{q},t) = \int d\mathbf{q}' K(\mathbf{q},\mathbf{q}',t)\psi(\mathbf{q}',0)$$

with

$$K(\mathbf{q},\mathbf{q}',t) = \sum_n \phi_n(\mathbf{q})e^{-iE_n t/\hbar}\phi_n^*(\mathbf{q}').$$

From the completeness relation, we obtain the boundary condition at $t = 0$:

$$\lim_{t\longrightarrow 0_+} K(\mathbf{q},\mathbf{q}',t) = \delta(\mathbf{q}-\mathbf{q}').$$

To obtain a semi-classical approximation to the propagator we follow now the ideas developed in last section. The only problem is that the initial condition demands that the propagator a $t = 0$ is a δ-funtion at $\mathbf{q} = \mathbf{q}'$, so our hypothetical cloud of particles is initially located at $\mathbf{q} = \mathbf{q}'$ with arbitrary velocity. However in the previous section we assumed that the particles at a certain point $\mathbf{q}$ have a defined velocity given by $\dot{q}_i = \partial_{p_i}H(\mathbf{q},\mathbf{p})$. This is the main reason why we will derive the semiclassical propagator considering it for short times first, and extrapolating from there to arbitrary times t.

3.1 Short times propagator

Away from $t = 0$ and for infinitesimally short times δt we write the propagator as,

$$K(\mathbf{q},\mathbf{q}',\delta t) = A(\mathbf{q},\mathbf{q}',\delta t)e^{\frac{i}{\hbar}R(\mathbf{q},\mathbf{q}',\delta t)}.$$

If the particle starts at $\mathbf{q} = \mathbf{q}' = (q_1', q_2', ..., q_d')$ and $\dot{\mathbf{q}} \approx (\mathbf{q}-\mathbf{q}')/\delta t$, the phase $R(\mathbf{q},\mathbf{q}',\delta t)$ is

$$R(\mathbf{q},\mathbf{q}',\delta t) = \frac{m}{2\delta t}(\mathbf{q}-\mathbf{q}')^2 - V(\mathbf{q})\delta t.$$

For infinitesimal times we can neglect the term $V(\mathbf{q})\delta t$, so $K_{sc}(\mathbf{q},\mathbf{q}',\delta t)$ could be considered as a d-dimensional Gaussian with width $\sigma^2 = i\hbar\delta t/m$. As we have seen, when t tends to zero, the propagator should be a Dirac delta. Thus, $A(\mathbf{q},\mathbf{q}',\delta t)$ is fixed by

$$\delta(\mathbf{z}) = \lim_{\sigma \longrightarrow 0} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\mathbf{z}^2/2\sigma^2},$$

and we obtain

$$K_{sc}(\mathbf{q},\mathbf{q}',\delta t) \approx (\frac{m}{2\pi i\hbar\delta t})^{\frac{3}{2}} e^{\frac{i}{\hbar}(\frac{m(\mathbf{q}-\mathbf{q}')^2}{2\delta t} - V(\mathbf{q})\delta t)}.$$

Also, the value of $\mathbf{p}$ at short times is

$$\mathbf{p} = \frac{\partial R}{\partial \mathbf{q}} \simeq \frac{m}{\delta t}(\mathbf{q}-\mathbf{q}').$$

We could reinterpret the prefactor $(m/\delta t)^{\frac{3}{2}}$ as the determinant of the Jacobian of the transformation from final position coordinates ($\mathbf{q}$) to the initial momentum coordinates ($\mathbf{p}'$), if we notice that

$$\frac{\partial p_i}{\partial q_j} = \frac{\partial}{\partial q_j}(\frac{\partial R}{\partial q_i'}) = -\frac{\partial^2 R}{\partial q_j \partial q_i'} = -\frac{\partial p_i'}{\partial q_j} = \frac{m}{\delta t}\delta_{ij}.$$

So the final expression for the semi-classical propagator at short times is

$$K_{sc}(\mathbf{q},\mathbf{q}',\delta t) = \frac{1}{(2\pi i\hbar)^{3/2}} (\det \frac{\partial \mathbf{p}'}{\partial \mathbf{q}})^{1/2} e^{\frac{i}{\hbar}(R(\mathbf{q},\mathbf{q}',\delta t)}, \tag{17}$$

where

$$\frac{\partial p_i'}{\partial q_j} \mid_{t,\mathbf{q}'} = \frac{\partial^2 R}{\partial q_j \partial q_i'}.$$

The subscript $...|_{t,\mathbf{q}'}$ indicates that the partial derivatives are evaluated with $\mathbf{q}'$ and t fixed.

In order to obtain the final expression we only have to evolve our short time approximation of the propagator according to (16)

$$K_{sc}(\mathbf{q}'',\mathbf{q}',t'+\delta t) = \sum_j |\det \frac{\partial \mathbf{q}}{\partial \mathbf{q}''}|_j^{1/2} \; e^{\frac{i}{\hbar}(R_j(\mathbf{q}'',\mathbf{q},t') - \frac{\pi}{2}\hbar m_j(\mathbf{q}'',\mathbf{q},t'))} K(\mathbf{q},\mathbf{q}',\delta t).$$

Here the topological index $m_j(\mathbf{q}'',\mathbf{q}',t)$ represents the number of singularities in the Jacobian along the j-th trajectory from $\mathbf{q}'$ to $\mathbf{q}''$. Here we have included the possibility that the phase becomes multi-valued, this is, that there are more than one path from $\mathbf{q}'$ to $\mathbf{q}''$.

If we take into account that $R(\mathbf{q}'',\mathbf{q}',t') + R(\mathbf{q},\mathbf{q}',\delta t) = R(\mathbf{q}'',\mathbf{q}',t'+\delta t)$ and also

$$\det \frac{\partial \mathbf{q}}{\partial \mathbf{q}''}|_t \; \det \frac{\partial \mathbf{p}'}{\partial \mathbf{q}}|_{\mathbf{q}',\delta t} = \det \frac{\partial \mathbf{p}'}{\partial \mathbf{q}''}|_{\mathbf{q}',t'+\delta t},$$

the final form of the semi-classical propagator (or *Van Vleck propagator*), is

$$K_{sc}(\mathbf{q},\mathbf{q}',t) = \sum_j \frac{1}{(2\pi i\hbar)^{3/2}} (\det \frac{\partial \mathbf{p}'}{\partial \mathbf{q}})^{1/2} \; e^{\frac{i}{\hbar}R(\mathbf{q},\mathbf{q}',t) - \frac{i}{2}\pi m_j}.$$

4 Semi-classical Green funtion

In the previous sections we have obtained approximate solutions to the time dependent Scrödinger equation and this solution remained valid for more complicated and time-dependent Hamiltonians. On the one hand, the propagator is important when we are interested in finite time quantum effects. On the other hand, and for time-independent Hamiltonian operators, the time dependence in the wave function and the propagator will be given in terms of the energy eigen-spectrum of the system as a given wave function can be expanded in energy eigen-basis

$$\psi(\mathbf{q},t)=\sum_n c_n e^{-iE_nt/\hbar}\phi_n(\mathbf{q})$$

and also the propagator

$$K(\mathbf{q},\mathbf{q}',t)=\sum_n \phi_n(\mathbf{q})e^{-iE_nt/\hbar}\phi_n^*(\mathbf{q}'),$$

Due to this fact, it is a good idea to change from a time to an energy representation, this is from the propagator to the Green's function. The semi-classical approximation of the Green's function $G_{sc}(\mathbf{q},\mathbf{q}',E)$ is the Laplace transform of the Van Vleck operator $K_{sc}(\mathbf{q},\mathbf{q}',t)$

$$G_{sc}(\mathbf{q},\mathbf{q}',E)=\frac{1}{i\hbar}\int_0^\infty dt\; e^{iEt/\hbar}K_{sc}(\mathbf{q},\mathbf{q}',t). \tag{18}$$

In order to evualate this integral we need to use the stationary phase method (Apendix I).

4.1 Green function for long trajectories

In order to evaluate the integral (18), in an approximate way, we have to distinguish between two types of contributions: one coming from stationary point of the phase and those coming from infinitesimally short times.

This is due to the singular behavior of the propagator for $t\longrightarrow 0$, where the amplitude does not change slowly compared with the phase.

Taking into account the form of the Van Vleck propagator, the stationary phase point (t^*) will be given by

$$\frac{\partial}{\partial t}R(\mathbf{q},\mathbf{q}',t^*)+E=0,$$

which is exactly the derivative with respect to time of the equation (15) so $t^*=t^*(\mathbf{q},\mathbf{q}',E)$ is the arbitrary time in which a particle goes from $\mathbf{q}'$ to $\mathbf{q}$, with a fixed energy E. And the second derivate evaluated at the stationary phase point is

$$R(\mathbf{q},\mathbf{q}',t)+Et=R(\mathbf{q},\mathbf{q}',t^*)+Et^*+\frac{1}{2}\frac{\partial^2}{\partial t^2}R(\mathbf{q},\mathbf{q}',t^*)(t-t^*)^2+...$$

So for a certain trajectory j in the Van Vleck propagator, the stationary phase approximation of the integral is

$$G_j(\mathbf{q},\mathbf{q}',E)=\frac{1}{i\hbar(2i\pi\hbar)^{(d-1)/2}}|\det C_j(\frac{\partial^2 R_j}{\partial t^2})^{-1}|^{1/2}e^{i(\frac{S_j}{\hbar}-m_j\frac{\pi}{2})}, \qquad (19)$$

where $C_j=\dfrac{\partial \mathbf{p}'}{\partial \mathbf{q}}$ and R_j are evaluated at time t^* and m_j includes now also the possible additional phase arising from the stationary phase integration.

First of all, we re-express the phase in terms of the action(which depends on energy)

$$S(\mathbf{q},\mathbf{q}',E)=R(\mathbf{q},\mathbf{q}',t^*)+Et^*, \quad with \quad t^*=t^*(\mathbf{q},\mathbf{q}',E)$$

and it is important to notice that the first derivative of the action respect to the coordinates is (*Cvitanovic* [2])

$$\frac{\partial S(\mathbf{q},\mathbf{q}',E)}{\partial \mathbf{q}}=\frac{\partial R(\mathbf{q},\mathbf{q}',t^*)}{\partial \mathbf{q}} \qquad (20)$$

Also, we will try to simplify the amplitude term in (19), rewriting it as a function of energy. Considering the matrix

$$D(\mathbf{q},\mathbf{q}',E)=\begin{bmatrix}\dfrac{\partial^2 S}{\partial \mathbf{q}\partial \mathbf{q}'} & \dfrac{\partial^2 S}{\partial E\partial \mathbf{q}'}\\ \dfrac{\partial^2 S}{\partial \mathbf{q}\partial E} & \dfrac{\partial^2 S}{\partial E^2}\end{bmatrix}=\begin{bmatrix}-\dfrac{\partial \mathbf{p}'}{\partial \mathbf{q}} & -\dfrac{\partial \mathbf{p}'}{\partial E}\\ \dfrac{\partial t}{\partial \mathbf{q}} & \dfrac{\partial t}{\partial E}\end{bmatrix}$$

taking into account the derivatives of (15) with respect to the energy and (14) with respect to the position

$$\frac{\partial}{\partial E}S(\mathbf{q},\mathbf{q}',E)=t$$

$$\frac{\partial}{\partial q_i'}S(\mathbf{q},\mathbf{q}',E)=p_i'.$$

Also is important to notice that the minus signs follow from the action definition (14), which implies that $S(\mathbf{q},\mathbf{q}',E)=-S(\mathbf{q}',\mathbf{q},E)$. It is easy to notice that, for a fixed $\mathbf{q}'$, D is the Jacobian matrix of the coordinate transformation $(\mathbf{q},E)\longrightarrow(\mathbf{p}',t)$.

$$\det D=(-1)^{d+1}[\det\frac{\partial(\mathbf{p}',t)}{\partial(\mathbf{q},E)}]_{\mathbf{q}'}=(-1)^{d+1}[\det\frac{\partial(\mathbf{p}',t)}{\partial(\mathbf{q},t)}\frac{\partial(\mathbf{q},t)}{\partial(\mathbf{q},E)}]_{\mathbf{q}'}$$

$$=(-1)^{d+1}(\det\frac{\partial \mathbf{p}'}{\partial \mathbf{q}})_{t,\mathbf{q}'}\,(\det\frac{\partial t}{\partial E})_{\mathbf{q}',\mathbf{q}}=\det C(\frac{\partial^2 R}{\partial t^2})^{-1}$$

In order to obtain this relation we have taken into account that

$$\frac{\partial^2 R}{\partial t^2}\frac{\partial^2 S}{\partial E^2}=\frac{\partial^2 R}{\partial t^2}\frac{\partial t}{\partial E}=-1.$$

We can now rewrite the semi-classical approximation of the contribution of the jth trajectory to the Green's function in explicity energy dependent form

$$G_j(q,q',E) = \frac{1}{i\hbar(2i\pi\hbar)^{(d-1)/2}} |\det D_j|^{1/2} e^{\frac{i}{\hbar}(S_j - \frac{\pi\hbar}{2}m_j)} \tag{21}$$

Taking into account that $G_j(\mathbf{q},\mathbf{q}',E)$ is constrained to a certain energy $H(\mathbf{q},\mathbf{p}=\frac{\partial S}{\partial \mathbf{q}}) = E$ we obtain

$$0 = \frac{\partial}{\partial \mathbf{q}} H(\mathbf{q},\mathbf{p}) = \sum_{j=1}^{d} \frac{\partial H}{\partial p_j}\frac{\partial p_j}{\partial \mathbf{q}} = \sum_{j=1}^{d} \frac{\partial^2 S}{\partial q_j \partial \mathbf{q}} \dot{q}_j$$

$$0 = \frac{\partial}{\partial \mathbf{q}} H(\mathbf{q}',\mathbf{p}') = \sum_{j=1}^{d} \frac{\partial H}{\partial p'_j}\frac{\partial p'_j}{\partial \mathbf{q}} = \sum_{j=1}^{d} \frac{\partial^2 S}{\partial \mathbf{q} \partial q'_j} \dot{q}'_j$$

Now we rotate the coordinate system to a new local configuration where the first coordinate ($q_\parallel$) is going to be always parallel to the trajectory and the rest $(d-1)$ perpendicular to it

$$(q_1, q_2, ..., q_d) \longrightarrow (q_\parallel, q_{\perp 1}, ..., q_{\perp(d-1)}),$$

also taking this into account, the velocity vector will be

$$(\dot{q}_1, \dot{q}_2, ..., \dot{q}_d) \longrightarrow (\dot{q}_\parallel, 0, ..., 0).$$

As the longitudinal coordinate axis $q_\parallel$ point always along the velocity vector of magnitude $\dot{\mathbf{q}}$, the matrix of $S(\mathbf{q},\mathbf{q}',E)$ has a column and a row of zeros because the initial and final velocities ($\dot{q}_\parallel$ and $\dot{q_\parallel}'$) are non-vanishing except for the turning points

$$0 = \dot{\mathbf{q}}' \frac{\partial^2 S}{\partial \mathbf{q} \partial q'_\parallel} = \dot{\mathbf{q}} \frac{\partial^2 S}{\partial q_\parallel \partial \mathbf{q}'}.$$

Evaluating also

$$\frac{\partial^2 S}{\partial q_\parallel \partial E} = \frac{\partial t}{\partial q_\parallel} = \frac{1}{\dot{q}_\parallel}$$

$$\frac{\partial^2 S}{\partial E \partial q'_\parallel} = \frac{\partial t}{\partial q'_\parallel} = \frac{1}{\dot{q_\parallel}'}$$

we can reduce the determinant of the [(d+1) x (d+1)] dimensional matrix

$$\det D(\mathbf{q},\mathbf{q}',E) = (-1)^{d+1} \det \begin{bmatrix} 0 & 0 & \frac{\partial^2 S}{\partial E \partial q'_\parallel} \\ 0 & \frac{\partial^2 S}{\partial \mathbf{q}_\perp \partial \mathbf{q}'_\perp} & * \\ \frac{\partial^2 S}{\partial q_\parallel \partial E} & * & * \end{bmatrix},$$

to the $[(d-1)\mathrm{x}(d-1)]$ dimensional transverse matrix $D_\perp(\mathbf{q},\mathbf{q}',E)$

$$\det D(q,q',E) = \frac{1}{\dot{q}_\parallel \dot{q}_\parallel{}'} \det D_\perp(\mathbf{q},\mathbf{q}',E)$$

$$D_\perp(\mathbf{q},\mathbf{q}',E)_{ik} = -\sum_{i=1}^{d-1}\sum_{k=1}^{d-1} \frac{\partial^2 S(q,q',E)}{\partial q_{\perp i}\partial q'_{\perp k}}.$$

Everything together for the jth trajectory is

$$G_j(\mathbf{q},\mathbf{q}',E) = \frac{1}{i\hbar(2i\pi\hbar)^{(d-1)/2}} \frac{1}{|\dot{q}_\parallel \dot{q}_\parallel{}'|^{1/2}} |\det D_\perp^j|^{1/2} \exp(\frac{i}{\hbar}S_j - \frac{i\pi}{2}m_j),$$

where m_j counts now the number of changes of sign of $\det D_\perp^j$ along the trajectory j which connects $\mathbf{q}'$ with $\mathbf{q}$ at energy E.

4.2 Green function for short trajectories

For short times we evaluate the integral involving the short time form of the exact quantum mechanical propagator (17).

$$G_0(\mathbf{q},\mathbf{q}',E) = \frac{1}{i\hbar}\int_0^\infty dt (\frac{m}{2it\pi\hbar})^{d/2} e^{\frac{i}{\hbar}([\frac{m(\mathbf{q}-\mathbf{q}')^2}{2t} - V(\mathbf{q})t] + Et)}$$

$$= \frac{m}{i\hbar^2(2i\pi)^{d/2}} (\frac{\sqrt{2m(E-V)}}{\hbar|\mathbf{q}-\mathbf{q}'|})^{\frac{d}{2}-1} \int_0^\infty \frac{d\tau}{\tau^{d/2}} e^{\frac{i}{2\hbar}S_0(\mathbf{q},\mathbf{q}',E)(\tau+1/\tau)},$$

where we have introduced the variable $\tau = \dfrac{\sqrt{2m(E-V)}}{\hbar|\mathbf{q}-\mathbf{q}'|}t$ and the action in the short distance form is $S_0 = \sqrt{2m(E-V)}|\mathbf{q}-\mathbf{q}|$.

Now if we use the integral representation of the Hankel function

$$H_\nu^+(z) = -\frac{i}{\hbar} e^{-i\nu\pi/2} \int_0^\infty e^{\frac{iz}{2}(\tau+1/\tau)} \tau^{-\nu-1} d\tau,$$

we can write the short distance form of the Green's function as

$$G_0(\mathbf{q},\mathbf{q}',E) \approx -\frac{im}{2\hbar^2} (\frac{\sqrt{2m(E-V)}}{2\hbar\pi|\mathbf{q}-\mathbf{q}'|})^{\frac{d-2}{2}} H^+_{\frac{d-2}{2}}(S_0/\hbar). \tag{22}$$

5 Trace formula and average density of states

As we are just interested in the spectra, our task is to evaluate the trace of the Green's function, this is formally talking,

$$TrG(\mathbf{q},\mathbf{q}',E) = \int dq\, G(\mathbf{q},\mathbf{q},E) = \int d^d q \sum_n \frac{\phi_n(\mathbf{q})\phi_n^*(\mathbf{q})}{E' + i\epsilon - E_n}$$

$$= \sum_n \frac{1}{E - E_n} \int d^d q \phi_n(\mathbf{q}) \phi_n^*(\mathbf{q}) = \sum_n \frac{1}{E - E_n},$$

defined in the half upper complex plane and $E = E' + i\epsilon$ is complex with imaginary positive part. In order to obtain this result we have taken into account the orthonormality of the basis for a bound systems $\int d^d q \ \phi_n(\mathbf{q}) \phi_m^*(\mathbf{q}) = \delta_{nm}$ and also the definition of the Green's function as the Laplace transform of the propagator. It is important to notice that this is only a formal trace because this sum is usually divergent.

The main reason to calculate this trace is that our final aim is to obtain the density of states, a representation with a delta peak at each eigen-energy.

$$d(E) = \sum_n \delta(E - E_n) = -\lim_{\epsilon \longrightarrow 0} \frac{1}{\pi} Im \ TrG(\mathbf{q}, \mathbf{q}', E' + i\epsilon), \tag{23}$$

where we have used the identity

$$\delta(E - E_n) = -\lim_{\epsilon \longrightarrow +0} \frac{1}{\pi} Im \ \frac{1}{E' - E_n + i\epsilon}.$$

5.1 Trace formula

So our task now is to evaluate the Green's function trace in the semi-classical approximation.

$$TrG_{sc}(E) = \int d^d q \, G_{sc}(\mathbf{q}, \mathbf{q}, E) = TrG_0(E) + TrG_{osc}(E) =$$

$$= TrG_0(E) + \sum_j \int d^d q \, G_j(\mathbf{q}, \mathbf{q}, E),$$

where there are contributions from the "zero length" trajectories, whose lengths approach to zero as $\mathbf{q}' \longrightarrow \mathbf{q}$, and the "long" classical ones, which start and end in q after a finite time.

We will begin with these last ones. As now we identify $\mathbf{q}$ with $\mathbf{q}'$,and perform the integral by using the stationary phase approximation.

$$\frac{\partial S_j(\mathbf{q}, \mathbf{q}', E)}{\partial q_i}|_{\mathbf{q}'=\mathbf{q}} + \frac{\partial S_j(\mathbf{q}, \mathbf{q}', E)}{\partial q_i'}|_{\mathbf{q}'=\mathbf{q}} = p_i(\mathbf{q}, \mathbf{q}, E) - p_i'(\mathbf{q}, \mathbf{q}, E) = 0,$$

so the trace receives contributions only from those long classical trajectories which are periodic in the full phase space (like positions, the initial and the final momenta coincide as well).

For a periodic orbit the natural coordinate system is the intrinsic one, with $q_\parallel$ axis pointing in the $\dot{q}$ direction along the orbit and the rest transverse to it. So, in this coordinates the jth periodic orbit contribution to the trace of the semi-classical Green's function is

$$TrG_j(E) = \frac{1}{i\hbar(2\pi\hbar)^{(3-1)/2}} \oint_j \frac{dq_\parallel}{\dot{q}} \int_j d\mathbf{q}_\perp |\det D_\perp^j|^{1/2} e^{\frac{i}{\hbar}(S_j - \frac{\hbar\pi}{2}m_j)},$$

where the integration in $q_\parallel$ goes from 0 to L_j. As always, in the stationary phase approximation we assume that the density varies smoothly so is well approximated by $D_\perp^j(q_\parallel, \mathbf{0}, E)$ on the classical trajectory, $\mathbf{q}_\perp = 0$. Also the topological index $m_j(q_\parallel, \mathbf{q}_\perp, E)$ does not depend on the initial point $q_\parallel$, so we set $m_j(E)$.

The transverse integration is carried out by the stationary phase method again, with the phase stationary on the periodic orbit, $\mathbf{q}_\perp = 0$. If we express the determinant of the second derivative matrix as

$$\det D'_{\perp j} = \det\left(\frac{\partial^2 S}{\partial q_{\perp i}\partial q_k} + \frac{\partial^2 S}{\partial q'_{\perp i}\partial q_k} + \frac{\partial^2 S}{\partial q_{\perp i}\partial q'_k} + \frac{\partial^2 S}{\partial q'_{\perp i}\partial q'_k}\right),$$

we obtain as a result of the transverse integration

$$TrG_j = \frac{1}{i\hbar} \oint \frac{dq_\parallel}{\dot{q}} \left|\frac{\det D_{\perp j}(q_\parallel, \mathbf{0}, E)}{\det D'_{\perp j}(q_\parallel, \mathbf{0}, E)}\right|^{1/2} e^{\frac{i}{\hbar}(S_j - \frac{\pi\hbar}{2}m_j)}.$$

So our next task is to obtain the value of $\det D_{\perp j}/\det D'_{\perp j}$. In terms of the monodromy matrix of the periodic orbit we could give to this determinant the next meaning

$$\det D_\perp = \left|\frac{\partial \mathbf{p}'_\perp}{\partial \mathbf{q}_\perp}\right| = \left|\frac{\partial \mathbf{q}'_\perp}{\partial \mathbf{q}_\perp}\frac{\partial \mathbf{p}'_\perp}{\partial \mathbf{q}'_\perp}\right| = \left|\frac{\partial(\mathbf{q}'_\perp, \mathbf{p}'_\perp)}{\partial(\mathbf{q}_\perp, \mathbf{q}'_\perp)}\right|$$

$$\det D'_\perp = \left|\frac{\partial \mathbf{p}_\perp}{\partial \mathbf{q}_\perp} - \frac{\partial \mathbf{p}'_\perp}{\partial \mathbf{q}_\perp} + \frac{\partial \mathbf{p}_\perp}{\partial \mathbf{q}'_\perp} - \frac{\partial \mathbf{p}'_\perp}{\partial \mathbf{q}'_\perp}\right| = \left|\frac{\partial(\mathbf{p}_\perp - \mathbf{p}'_\perp, \mathbf{q}_\perp - \mathbf{q}'_\perp)}{\partial(\mathbf{q}'_\perp, \mathbf{q}_\perp)}\right|,$$

and defining the transverse vector $\mathbf{x}_\perp = (\mathbf{q}_\perp, \mathbf{p}_\perp)$ in the full phase space, the ratio is now

$$\frac{\det D'_\perp}{\det D_\perp} = \left|\frac{\partial(\mathbf{p}_\perp - \mathbf{p}'_\perp, \mathbf{q}_\perp - \mathbf{q}'_\perp)}{\partial(\mathbf{q}'_\perp, \mathbf{q}_\perp)}\right| \left|\frac{\partial(\mathbf{q}_\perp, \mathbf{q}'_\perp)}{\partial(\mathbf{q}'_\perp, \mathbf{p}'_\perp)}\right| = \left|\frac{\partial(\mathbf{p}_\perp - \mathbf{p}'_\perp, \mathbf{q}_\perp - \mathbf{q}'_\perp)}{\partial(\mathbf{q}'_\perp, \mathbf{p}'_\perp)}\right|$$

$$= \left|\frac{\partial(\mathbf{x}_\perp - \mathbf{x}'_\perp)}{\partial \mathbf{x}'_\perp}\right| = \det(\mathsf{M} - 1),$$

where M is the monodromy matrix for a surface of section transverse orbit within the constant energy $E = H(\mathbf{q}, \mathbf{p})$ shell.

Furthermore, the classical periodic orbit action $S_j(E)$ is an integral around the loop defined by the periodic orbit, but does not depend on the starting point $q_\parallel$, and is defined as

$$S_j(E) = \oint p(q_\parallel, E) dq_\parallel,$$

as M neither depends on it, the action and the term $\det(1-\mathsf{M}_j)$ can be taken out of the $q_\parallel$ integral

$$trG_j(E) = \frac{1}{i\hbar}\sum_j \frac{1}{|\det(1-\mathsf{M}_j)|^{1/2}} e^{\frac{i}{\hbar}(S_j - \frac{\hbar\pi}{2}m_j)} \oint \frac{dq_\parallel}{\dot{q}}.$$

Here we have assumed that M_j has no marginal values. The action $S_j(E)$, the topological index m_j and M_j are classical invariants of the periodic orbit.

Taking into account the fact that any repeat of a periodic orbit is also a periodic orbit and as the action and the topological index are additive along the trajectory, for rth repeat we simply multiply by r. Also, because of the chain rule of derivatives, the monodromy matrix of the rth repeat of a prime cycle p is simply $(\mathsf{M}_\mathrm{p})^r$, where M_p is the prime cycle monodromy matrix.

Now we denote the time period of the prime cycle p, the single transversal of a periodic by T_p. As $dt = dq_\parallel/\dot{q}(t)$

$$\int_0^{L_\mathrm{p}} \frac{dq_\parallel}{\dot{q}(t)} = \int_0^{T_\mathrm{p}} dt = T_\mathrm{p}.$$

All in all, we obtain the *Gutzwiller trace formula*

$$TrG_{sc} = TrG_0 + \frac{1}{i\hbar}\sum_\mathrm{p} T_\mathrm{p} \sum_{r=1}^{\infty} \frac{1}{|\det(1-\mathsf{M}_\mathrm{p}^r)|^{1/2}} e^{\frac{ir}{\hbar}(S_\mathrm{p} - \frac{\hbar\pi}{2}m_\mathrm{p})} \qquad (24)$$

where the topological index $m_\mathrm{p}(E)$ counts the number of changes of sign of the second derivatives evaluated along the periodic orbit p. (24) is valid only for isolated periodic orbits as occurs in 1d systems and chaotic systems.

5.2 Average density of states

The semi-classical contribution to the density of states is given by the imaginary part of the Gutzwiller formula (24) multiplied with -1/π. Also the contribution coming from zero length trajectories is the imaginary part of (22) for $q' \to q$ integrated over the configuration space

$$d_0(E) = -\frac{1}{\pi}\int d\mathbf{q} ImG_0(\mathbf{q},\mathbf{q},E),$$

and coincides with the classical value of the density of states, whose expression is in general

$$d_0(E) = \int \frac{d\mathbf{p}d\mathbf{q}}{(2\pi\hbar)^d}\delta(E - H(\mathbf{q},\mathbf{p}))$$

The final form for the semi-classical density of states is a sum of this average density and the oscillation density of states around the average, derived from the second part of (24), $d_{sc}(E) = d_0(E) + d_{osc}(E)$ where

$$d_{osc} = \frac{1}{\pi\hbar}\sum_\mathrm{p} T_\mathrm{p} \sum_{r=1}^{\infty} \frac{cos(rS_\mathrm{p}(E)/\hbar - rm_\mathrm{p}\pi/2)}{|\det(1-\mathsf{M}_\mathrm{p}^r)|^{1/2}}$$

Part II
Application

Ahora, partiendo del formalismo anteriormente desarrollado, procederemos a la resolución de un problema concreto. Este consistirá en un sistema de una sola partícula unidimensional atrapada en un potencial cúbico.

El primer paso para el cálculo de las acciones y periodos tanto en la barrera como en el pozo es obtener los puntos en los que el potencial se anula para cada valor de la energía. Además, como hemos visto en la sección anterior, a la traza contribuirán todas las posibles trayectorias cerradas, tanto reales como imaginarias y tendremos que considerarlas a la hora de obtener la misma.

Finalmente, mediante teoría de perturbaciones , obtenemos las correcciones a las auto-energías a orden cero, de la que recuperaremos la condición de cuantización de Bohr-Sommerfeld, y a primer orden, que podremos relacionar con el tiempo de vida de los estados.

6 Cubic potential problem

Our next step is to use this formalism in a particular case. We will study the semi-classical dynamics of a particle with mass m under the effect of a cubic potential in 1d configuration space. This potential will have a relative minimum at $q = 0$, and a relative maximum, this is, a potential barrier.

The Hamiltonian operator for this system in the coordinate (q) representation is

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial q^2} + \frac{1}{2}kq^2 - \alpha q^3.$$

Performing now the coordinate change

$$q = aq_*,$$

which leads us to

$$\hat{H} = -\frac{\hbar^2}{2ma^2}\frac{\partial^2}{\partial q_*^2} + \frac{1}{2}ka^2q_*^2 - \alpha a^3 q_*^3.$$

Choosing a so that

$$ka^2 = \frac{\hbar^2}{ma^2}$$

which gives

$$a = \sqrt{\frac{\hbar}{\sqrt{mk}}}.$$

Now, scaling $\hat{H}$ in the form

$$\hat{H} = ka^2\hat{H}',$$

where the scaled Hamiltonian operator is then

$$\hat{H}' = \frac{\hat{H}}{\hbar\omega_0} = -\frac{1}{2}\frac{\partial^2}{\partial q_*^2} + \frac{1}{2}q_*^2 - \alpha_* q_*^3,$$

where $\omega_0 = \sqrt{\frac{k}{m}}$ is the frequency at the minimum of the potential and α_* is the only parameter of the problem. $\hat{H}'$ measures energy in units of $\hbar\omega_0$, and is a reduced Hamiltonian operator in which $\hbar = 1$.

Now,with $q_* \equiv q$ the classical Hamiltonian operator will be

$$H = \frac{p^2}{2} + \frac{q^2}{2} - \alpha_* q^3.$$

First of all, we want to re-express the constant α_* in the potential $V(q) = \frac{q^2}{2} - \alpha_* q^3$ as a function of D, the energy at the barrier top. If we take into account that, when we are at the top of our potential

$$\frac{\partial V}{\partial q} = q - 3\alpha_* q^2 = 0,$$

this leads us to

$$q_m = \frac{1}{3\alpha_*}.$$

Now in order to obtain the relation between α_* and D, we substitute this q_m value in $V(q)$

$$V(q_m) = D = \frac{1}{2}(\frac{1}{3\alpha_*})^2 - \alpha_*(\frac{1}{3\alpha_*})^3 = \frac{1}{9\alpha_*^2}(\frac{1}{2} - \frac{1}{3}) = \frac{1}{54\alpha_*^2}.$$

Taking this into account, the final expression for the potential will be

$$V(q) = \frac{q^2}{2} - \frac{q^3}{\sqrt{54D}},$$

which fulfills

$$\lim_{q \longrightarrow -\infty} V(q) = +\infty$$

$$\lim_{q \longrightarrow \infty} V(q) = -\infty.$$

A plot of this potential is given in Figure 1.

Taking these conditions into account we will have a non-degenerate continuous spectrum (*Cohen-Tannoudji, Diu and Laloe* [3]).

We will study our system for energies $0 < E < D$, i.e., within the potential well region. As far as the spectrum is concerned, there is a certain probability of trapped states within the barrier, which decay through tunelling

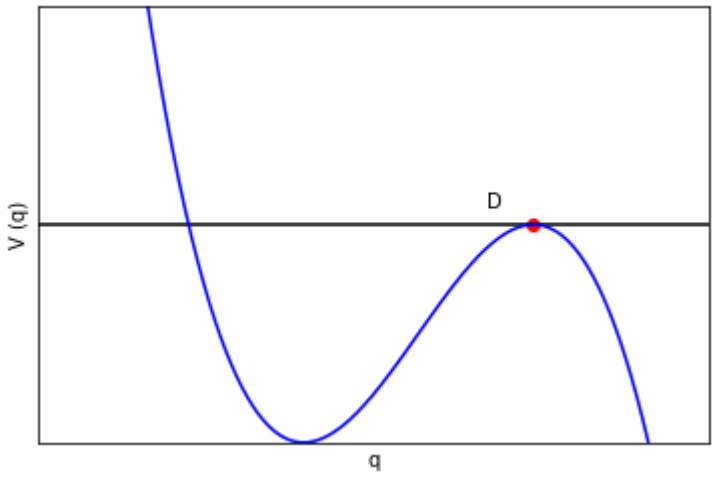

Figure 1: Potential V(q)

across the barrier. These states are called resonances in scattering theory and are immersed in the continuous spectrum.

One can associate a complex energy with them

$$E = E_r - iE_i.$$

The imaginary part is responsible for the decay of the state into the continuum.

The rate of this decay will be

$$\Gamma = \frac{2E_i}{\hbar},$$

and the lifetime

$$\tau = \frac{1}{\Gamma}.$$

Since we want to obtain, for the different values of the energy (E), the three points where the potential cuts the q-axis, we make $p = 0$ and then

$$p = \sqrt{2(E - V)} = 0 \Rightarrow 2(E - V) = 0,$$

so the final equation which we have to solve is

$$\frac{2}{\sqrt{54D}}q^3 - q^2 + 2E = 0$$

This equation depends on E as a parameter and we are going to find its solutions using the *Cardano's Method*. This method allows us to solve analytically any cubic equation in one variable. So for an equation like

$$\alpha x^3 + \beta x^2 + \gamma x + \delta = 0$$

where α, β, γ, and δ are real numbers, we first divide the whole equation by the coefficient α so we obtain

$$x^3 + ax^2 + bx + c = 0.$$

and in our problem $a = -\sqrt{\frac{27D}{2}}$, $b = 0$ and $c = \sqrt{54D}E$.

Now we are going to obtain the *reduced form* of the cubic equation

$$z^3 + pz + q = 0$$

where

$$z = x + \frac{a}{3} = x - \frac{3}{2}\sqrt{54D},$$

$$p = b - \frac{a^2}{3} = -\frac{9D}{2},$$

$$q = \frac{2a^3}{27} - \frac{ab}{3} + c = -\sqrt{\frac{27D}{2}} + \sqrt{54D}E.$$

Taking into account the value of the discriminant $\Delta = (q/2)^2 + (p/3)^3$ it is easy to calculate one of the roots as

$$x = \sqrt[3]{-\frac{q}{2} + \sqrt{\Delta}} + \sqrt[3]{-\frac{q}{2} - \sqrt{\Delta}} - \frac{a}{3}$$

Once this root is obtained (for each value of E) it is simple to calculate the other two using Ruffini's rule.

To study this problem we need, not only real trajectories, but also imaginary ones in order to describe the tunnelling.

For a general Hamiltonian operator

$$H = \frac{p^2}{2} + V(q),$$

the Hamilton's equations will be

$$\dot{q} = p$$

$$\dot{p} = -\frac{\partial V}{\partial q}$$

As the momentum p is

$$p = \pm\sqrt{2(E - V)} = \frac{dq}{dt} \tag{25}$$

we can obtain the time necessary to go from q' to q as

$$t = \int_{q'}^{q} \frac{dq}{\pm\sqrt{2(E - V)}}. \tag{26}$$

Here, we have two different possibilities. When $E > D$, this is, when the movement of the particle takes place over the barrier, $2(E - V) > 0$, which implies that, not only q, p and t are always real, but also the trajectories. However, when $E < D$, which is the case we are dealing with, we will have real and imaginary trajectories. In the well, where $E > V$, q, p ,t and the trajectories will be real, but below the barrier, as $E < V$, q remains real but t and p, according to (25) and (26), will both be imaginary. This leads us to a complex trajectory, which means that, when we enter the barrier we are increasing the imaginary parts of the time (t) and the momentum (p), and when we enter the well, their real parts.

In this region, performing now the changes

$$p \to ip'$$

$$t \to -it'$$

$$q \to q',$$

where p' and t' are now real.

The Hamilton's equations are then

$$\frac{dq'}{dt'} = p'$$

$$\frac{dp'}{dt'} = \frac{\partial V}{\partial q'},$$

and the new Hamiltonian operator

$$H' = \frac{p'^2}{2} - V(q'),$$

so, by performing this change, we have real trajectories in a reversed potential.

Taking this into account, we are going to evaluate actions and periods in two regions (Γ and Γ_b). These periods and actions will be calculated from the periodic trajectories with their beginnings and ends in the well and the barrier. Also, we will denote as S the real action of the periodic orbits at energy E in the well and S_b the imaginary action of a round-trip oscillation under the potential barrier.

Now, we are going to write the trace of the Green's function as an addition over all the real and imaginary periodic trajectories which begin in any of these two regions. Keeping in mind all the possibilities we will follow the procedure followed by *Martín-Fierro* [4] in the resolution of another problem. It is important to remember that the only trajectories which contribute to the trace of the Green's function are the periodic ones, also called orbits, as we said in (24).

First, we are going to study the trajectories which start below the barrier. In the case in which the particle starts in a point under the barrier and goes back after a certain number of laps in the well

$$-e^{S_b/\hbar}\sum_{l=0}^{\infty}(-e^{iS/\hbar})^l.$$

Another possibility is a similar process, but performing two passes down the barrier instead of one

$$e^{-S_b/2\hbar}\sum_{l=0}^{\infty}(-e^{iS/\hbar})^l(-e^{-S_b/2\hbar})e^{-S_b/2\hbar}\sum_{l=0}^{\infty}(-e^{iS/\hbar})^l(-e^{-S_b/2\hbar})$$

$$=[(-e^{-S_b/\hbar})\sum_{l=0}^{\infty}(-e^{iS/\hbar})^l]^2$$

And all the trajectories which start and end below the barrier will be then characterized by

$$\sum_{n=1}^{\infty}[(-e^{-S_b/\hbar})\sum_{l=0}^{\infty}(-e^{iS/\hbar})^l]^n.$$

On the other hand, as far as the trajectories which start in the well is concerned, we should take into account that here we could make infinite oscillations in the well without leaving it

$$\sum_{n=1}^{\infty}(-e^{iS/\hbar})^n,$$

and if the particle also makes a round-trip oscillation within the barrier

$$\sum_{n=1}^{\infty}(-e^{iS/\hbar})^n(-e^{-S_b/2\hbar})e^{-S_b/2\hbar}\sum_{l=0}^{\infty}(-e^{iS/\hbar})^l=\sum_{n=1}^{\infty}(-e^{iS/\hbar})^n e^{-S_b/\hbar}\sum_{l=0}^{\infty}(-e^{iS/\hbar})^l.$$

For two laps under the barrier

$$\sum_{n=1}^{\infty}(-e^{iS/\hbar})^n(-e^{-S_b/\hbar})\sum_{l=0}^{\infty}(-e^{iS/\hbar})^l(-e^{-S_b/2\hbar})e^{-S_b/2\hbar}\sum_{l=0}^{\infty}(-e^{iS/\hbar})^l=$$

$$=\sum_{n=1}^{\infty}(-e^{iS/\hbar})^n[(-e^{-S_b/\hbar})\sum_{l=0}^{\infty}(-e^{iS/\hbar})^l]^2.$$

Taking this into account, all the trajectories which begin at the well will be characterized by

$$\sum_{n=1}^{\infty}(-e^{iS/\hbar})^n\sum_{j=0}^{\infty}[(-e^{-S_b/\hbar})\sum_{l=0}^{\infty}(-e^{iS/\hbar})^l]^j.$$

These two cases lead us to a trace of the Green's functions with the next shape

$$TrG_{osc}(E) = \frac{1}{i\hbar}(\sum_{n=1}^{\infty}[(-e^{-S_b/\hbar}) \sum_{l=0}^{\infty}(-e^{iS/\hbar})^l]^n \int_{\Gamma_b} dq \frac{1}{\dot{q}} +$$

$$+ \sum_{n=1}^{\infty}(-e^{iS/\hbar})^n \sum_{j=0}^{\infty}[(-e^{-S_b/\hbar}) \sum_{l=0}^{\infty}(-e^{iS/\hbar})^l]^j \int_{\Gamma} dq \frac{1}{\dot{q}})$$

$$= \frac{1}{i\hbar}(-iT_b \sum_{n=1}^{\infty}[(-e^{-S_b/\hbar}) \sum_{l=0}^{\infty}(-e^{iS/\hbar})^l]^n + T \sum_{n=1}^{\infty}(-e^{iS/\hbar})^n \sum_{j=0}^{\infty}[(-e^{-S_b/\hbar}) \sum_{l=0}^{\infty}(-e^{iS/\hbar})^l]^j)$$

If we keep in mind the geometrical series

$$\sum_{n=0}^{\infty} x^n = \frac{1}{1-x},$$

and we apply it to the terms of our trace formula:

$$\sum_{l=0}^{\infty}(-e^{iS/\hbar})^l = \frac{1}{1+e^{iS/\hbar}},$$

what we obtain is

$$TrG_{osc}(E) = \frac{1}{i\hbar}[-iT_b \sum_{n=1}^{\infty}(\frac{-e^{-S_b\hbar}}{1+e^{iS/\hbar}})^n + T \sum_{n=1}^{\infty}(-e^{iS/\hbar})^n \sum_{j=0}^{\infty}(\frac{-e^{-S_b/\hbar}}{1+e^{iS/\hbar}})^j].$$

Now we are going to treat these three additions separately

$$\sum_{n=1}^{\infty}(\frac{-e^{-S_b\hbar}}{1+e^{iS/\hbar}})^n = \frac{1}{1+\frac{e^{-S_b\hbar}}{1+e^{iS/\hbar}}} - 1 = \frac{1+e^{iS/\hbar}}{1+e^{iS/\hbar}+e^{-S_b\hbar}} - 1 = \frac{-e^{-S_b\hbar}}{1+e^{iS/\hbar}+e^{-S_b\hbar}}$$

$$\sum_{n=1}^{\infty}(-e^{iS/\hbar})^n = \frac{1}{1+e^{iS/\hbar}} - 1 = \frac{-e^{iS/\hbar}}{1+e^{iS/\hbar}}$$

$$\sum_{j=0}^{\infty}(\frac{-e^{-S_b/\hbar}}{1+e^{iS/\hbar}})^j = \frac{1}{1+\frac{-e^{-S_b/\hbar}}{1+e^{iS/\hbar}}} = \frac{1+e^{iS/\hbar}}{1+e^{iS/\hbar}+e^{-S_b\hbar}},$$

and because of this

$$TrG_{osc}(E) = \frac{1}{i\hbar}[\ \frac{iT_b e^{-S_b\hbar} - Te^{iS/\hbar}}{1+e^{iS/\hbar}+e^{-S_b\hbar}}\ ] \tag{27}$$

The contribution of the *zero length* is easy to obtain. We just calculate it as the half of the terms corresponding to the zero order term in the TrG_{osc} expression, so we finally obtain:

$$TrG(E) = \frac{T-iT_b}{2i\hbar} + \frac{1}{i\hbar}[\ \frac{iT_b e^{-S_b\hbar} - Te^{iS/\hbar}}{1+e^{iS/\hbar}+e^{-S_b\hbar}}\ ], \tag{28}$$

where $T = \dfrac{\partial S}{\partial E}$ and $T_b = -\dfrac{\partial S_b}{\partial E}$ are the periods in the well and the barrier. The integrals to calculate the periods and the actions (S and S_b) are

$$S = 2\int_{x_1}^{x_2} dx\sqrt{2(E-V)} = 2\sqrt{\frac{2}{\sqrt{54D}}}\int_{x_1}^{x_2} dx\sqrt{(x-x_1)(x-x_2)(x-x_3)}$$

$$S_b = 2\int_{x_2}^{x_3} dx\sqrt{2(E-V)} = 2\sqrt{\frac{2}{\sqrt{54D}}}\int_{x_2}^{x_3} dx\sqrt{(x-x_1)(x-x_2)(x-x_3)}$$

$$T = 2\int_{x_1}^{x_2} \frac{dx}{\sqrt{2(E-V)}} = 2\sqrt{\frac{\sqrt{54D}}{2}}\int_{x_1}^{x_2} \frac{dx}{\sqrt{(x-x_1)(x-x_2)(x-x_3)}}$$

$$T_b = 2\int_{x_2}^{x_3} \frac{dx}{\sqrt{2(E-V)}} = 2\sqrt{\frac{\sqrt{54D}}{2}}\int_{x_2}^{x_3} \frac{dx}{\sqrt{(x-x_1)(x-x_2)(x-x_3)}},$$

where x_1, x_2 and x_3 are the three turning points of our cubic potential with $(x_1 \leq x_2 \leq x_3)$.

First of all, we are going to calculate the action in the well (S):

$$S = 2\sqrt{\frac{2}{\sqrt{54D}}}\int_{x_1}^{x_2} dx\sqrt{(x-x_1)(x-x_2)(x-x_3)} =$$

$$= 2\sqrt{\frac{2}{\sqrt{54D}}}\int_{x_1}^{x_2} dx\sqrt{(x-x_1)(x_2-x)(x_3-x)}.$$

If we perform the next variable change:

$$y = x - a,$$

we obtain

$$S = 2\sqrt{\frac{2}{\sqrt{54D}}}\int_{0}^{x_2-x_1} dx\sqrt{y\ (x_2-x_1-y)(x_3-x_1-y)},$$

and then a second variable change:

$$y = (x_2-x_1)z,$$

leads us to

$$S = 2\sqrt{\frac{2}{\sqrt{54\ D}}}\sqrt{x_3-x_1}\ (x_2-x_1)^2\int_{0}^{1} dz\sqrt{z(1-z)(1-\frac{x_2-x_1}{x_3-x_1}z)}.$$

Taking into account (*Gradshteyn, Ryzhik, Tseytlin*[5])

$$\int_0^1 x^{\lambda-1}(1-x)^{\mu-1}(1-\beta x)^{-\nu}dx = B(\lambda,\mu)\ {}_2F_1(\nu,\lambda;\lambda+\mu;\beta),$$

where $B(\lambda,\mu)$ is the Beta function and ${}_2F_1(\nu,\lambda;\lambda+\mu;\beta)$ is a hypergeometric function, we obtain

$$S = 2\sqrt{\frac{2}{\sqrt{54D}}}\sqrt{x_3-x_1}\,(x_2-x_1)^2 B(\frac{3}{2},\frac{3}{2})\;{}_2F_1(\frac{3}{2},-\frac{1}{2},3;\frac{x_2-x_1}{x_3-x_1}).$$

Following this same procedure we can obtain T, S_b and T_b

$$T = 2\int_{x_1}^{x_2}\frac{dx}{\sqrt{2(E-V)}} = 2\sqrt{\frac{\sqrt{54D}}{2}}\int_{x_1}^{x_2}\frac{dx}{\sqrt{(x-x_1)(x-x_2)(x-x_3)}}$$

$$= 2\sqrt{\frac{\sqrt{54D}}{2}}\frac{1}{\sqrt{x_2-x_1}}\frac{1}{\sqrt{x_2-x_1}}\frac{1}{\sqrt{x_3-x_1}}\,(x_2-x_1)\int_0^1 dz\frac{1}{\sqrt{z(1-z)(1-\frac{x_2-x_1}{x_3-x_1}z)}}$$

$$= \frac{\sqrt[4]{54D}}{2}\frac{1}{\sqrt{x_3-x_1}}\,B(\frac{1}{2},\frac{1}{2})\;{}_2F_1(\frac{1}{2},\frac{1}{2},1;\frac{x_2-x_1}{x_3-x_1}).$$

$$S_b = 2\sqrt{\frac{2}{\sqrt{54D}}}\sqrt{x_2-x_1}\,(x_3-x_2)^2 B(\frac{3}{2},\frac{3}{2})\;{}_2F_1(\frac{3}{2},-\frac{1}{2},3;\frac{x_3-x_2}{x_1-x_2})$$

$$T_b = \frac{\sqrt[4]{54D}}{2}\frac{1}{\sqrt{x_2-x_1}}\,B(\frac{1}{2},\frac{1}{2})\;{}_2F_1(\frac{1}{2},\frac{1}{2},1;\frac{x_3-x_2}{x_1-x_2}).$$

We are going to obtain now an approximation to the complex energies of the resonances. From the previous analysis we know that the trace of the Green's function shows singularities or poles at the energies of the discrete spectrum. If we have a continuous spectrum, these poles will correspond to resonances. From (27), these poles correspond to the zeros of the denominator, i.e.

$$1 + e^{iS/\hbar} = -\varepsilon e^{-S_b/\hbar},$$

where we have proceeded in a perturbative way, introducing a parameter (ε), to explicitly show the smallness of $e^{-S_b/\hbar}$.

If we made a series expansion of the eigen-energies as powers of ε

$$E_n = E_n^{(0)} + \varepsilon E_n^{(1)} + \varepsilon^2 E_n^{(2)} + ...$$

and we expand both actions around $E_n^{(0)}$

$$S(E_n) \simeq S(E_n^{(0)}) + \frac{\partial S}{\partial E_n}|_{E_n^{(0)}}(E_n - E_n^{(0)}) + \frac{1}{2}\frac{\partial^2 S}{\partial E_n^2}|_{E_n^{(0)}}(E_n - E_n^{(0)})^2 =$$

$$= S(E_n^{(0)}) + T(\varepsilon E_n^{(1)} + \varepsilon^2 E_n^{(2)}) + \frac{1}{2}\frac{\partial T}{\partial E_n}|_{E_n^{(0)}}(E_n^{(1)})^2$$

$$S_b(E_n) \simeq S_b(E_n^{(0)}) - T_b(E_n - E_n^{(0)}) - \frac{\varepsilon^2}{2}\frac{\partial T_b}{\partial E_n}|_{E_n^{(0)}}(E_n - E_n^{(0)})^2 =$$

$$= S_b(E_n^{(0)}) - T_b(\varepsilon E_n^{(1)} + \varepsilon^2 E_n^{(2)}) - \frac{\varepsilon^2}{2}\frac{\partial T_b}{\partial E_n}|_{E_n^{(0)}}(E_n^{(1)})^2$$

to finally substitute them in the pole condition

$$1 + e^{\frac{i}{\hbar}S(E_n^{(0)})} e^{\frac{iT}{\hbar}(\varepsilon E_n^{(1)} + \varepsilon^2 E_n^{(2)})} e^{\frac{i}{2\hbar}\frac{\partial T}{\partial E_n}(E_n^{(1)})^2} =$$

$$= -\varepsilon e^{-\frac{S_b}{\hbar}(E_n^{(0)})} e^{\frac{T_b}{\hbar}(\varepsilon E_n^{(1)} + \varepsilon^2 E_n^{(2)})} e^{\frac{1}{2\hbar}\frac{\partial T_b}{\partial E_n}|(\varepsilon E_n^{(1)})^2} \tag{29}$$

Our next step is to apply the McLaurin series to the exponentials in (29)

$$e^x = \sum_{k=0}^{\infty} \frac{x^k}{k!} = 1 + x + \frac{x^2}{2} + ... + \frac{x^n}{n!}$$

with it, up to second order, we obtain

$$1 + e^{\frac{i}{\hbar}S(E_n^{(0)})}[1 + \frac{iT}{\hbar}(\varepsilon E_n^{(1)} + \varepsilon^2 E_n^{(2)}) - \frac{T^2}{2\hbar}(\varepsilon E_n^{(1)})^2][1 + \frac{i}{2\hbar}\frac{\partial T}{\partial E_n}(\varepsilon E_n^{(1)})^2] =$$

$$= -\varepsilon e^{-S_b(E_n^{(0)})}[1 + \frac{T_b}{\hbar}(\varepsilon E_n^{(1)} + \varepsilon^2 E_n^{(2)}) + \frac{T_b^2}{2\hbar}(\varepsilon E_n^{(1)})^2][1 + \frac{1}{2\hbar}\frac{\partial T}{\partial E_n}(\varepsilon E_n^{(1)})^2].$$

Now if we indentify the coefficients at each order of ε. At zero order

$$1 + e^{\frac{i}{\hbar}S(E_n^{(0)})} = 0 \tag{30}$$

we obtain the Bohr-Sommerfeld quantization condition (8)

$$S(E_n^{(0)}) = (2n+1)\pi\hbar.$$

At first order

$$1 + e^{\frac{i}{\hbar}S(E_n^{(0)})}[1 + \frac{iT}{\hbar}(\varepsilon E_n^{(1)})] = -\varepsilon e^{-S_b(E_n^{(0)})}$$

$$1 + e^{\frac{i}{\hbar}S(E_n^{(0)})} + \frac{iT}{\hbar}(\varepsilon E_n^{(1)}) e^{\frac{i}{\hbar}S(E_n^{(0)})} = -\varepsilon e^{-S_b(E_n^{(0)})}$$

Taking into account (30)

$$\frac{i}{\hbar}T E_n^{(1)} = e^{-S_b(E_n^{(0)})}$$

$$E_n^{(1)} = \frac{\hbar}{iT} e^{-S_b(E_n^{(0)})} \tag{31}$$

So, this leads us to a correction to the zero order eigen-energies

$$E_n \simeq E_n^{(0)} - \frac{i\hbar}{T} e^{-S_b(E_n^{(0)})}, \tag{32}$$

and the rate is then

$$\frac{\Gamma}{2} = \frac{e^{-S_b(E_0)/\hbar}}{T} \tag{33}$$

Now we will show some plots of the magnitudes that are relevant in this problem. Figure 2 plots the actions in the well (S) and under the barrier (S_b) for a height of the barrier $D = 2.5$. As it is expected, the action in the well (S) with E increases, while the action under the barrier (S_b) decreases. Figure 3 gives the periods of the real periodic orbit in the well (T) and the complex periodic orbit (T_b) under the barrier as a function of E. One can check these periods are the derivatives of the action in figure 2 with respect to the energy (E). These periods go to infinity either at $E = 0$ or $E = D$. In these plots, and for the density of states represented in figure 6, we have used 10000 points from $E = 0$ to $E = D = 2.5$. The calculation needed to obtain the results of this project have been performed using a python lenguage program.

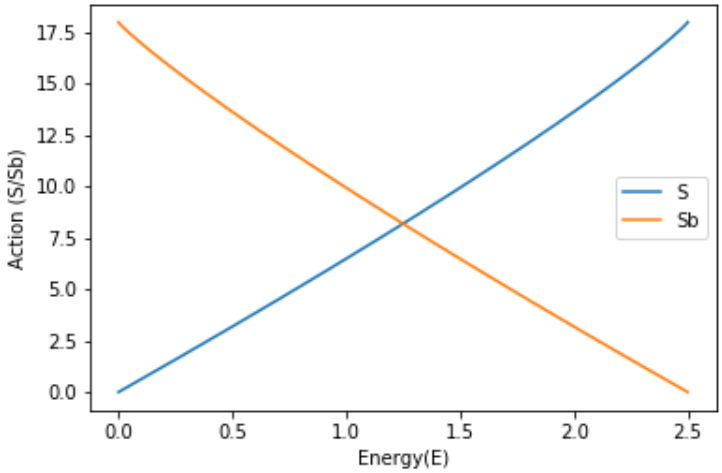

Figure 2: Actions in the well and below the barrier for D=2.5

There is an upper bound for the number of resonances we can find for a D value. Using the Bohr-Sommerfield quantization condition (8), with $\hbar = 1$

$$S(E) = 2\pi(n + \frac{1}{2})$$

we can find the n value for $E = D$, which is the maximum n value in the well. From this value of n, we can obtain the maximun number of resonaces in the well (N) as

$$N = n + 1 = (\frac{S(D)}{2\pi} - \frac{1}{2}) + 1 = \frac{S(D)}{2\pi} + \frac{1}{2}$$

For example, as can be seen in figure 6, in the particular case of $D = 2.5$ we have three resonaces, while for $D = 4.5$, as we can see in figure 7, we have five.

Now we will use the Bohr-Sommerfield quatization condition (8) and (32) to find complex energies of the quantum resonaces. With this objective, we will use a root finder routine to find $E_n^{(0)}$ and then we apply it to (31) in order to obtain the imaginary part of the energy ($E_n^{(1)}$). In figures 4 and 5 we give

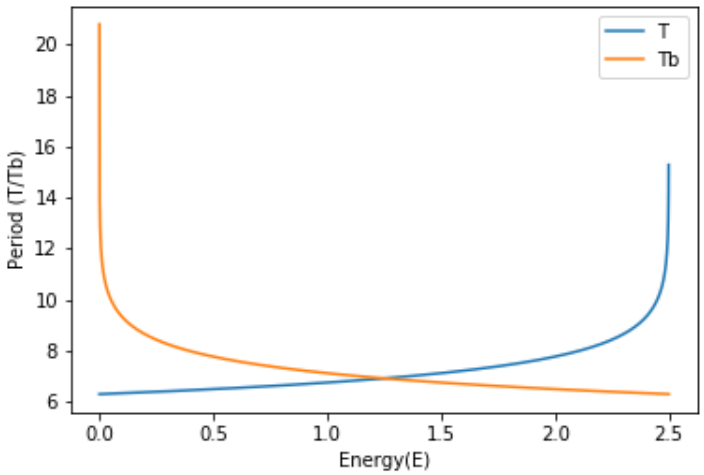

Figure 3: Periods in the well and below the barrier for D=2.5

the value of the complex energy (E) of the resonances for each n value in both examples.

n	E_r	E_i
0	0.492727896	1.740996123 x 10^{-7}
1	1.426667582	0.000131463
2	2.256795658	0.025419448

Figure 4: Values of the real (E_r) and the imaginary (E_i) part of the Energy (E) for each n in the case $D = 2.5$.

As n increases, the magnitude of the imaginary part of the energy increases too, and as S_b decreases (see figure 2),and taking into account the expresion for the ratio (33), the tunelling probability increases and the resonant states decay faster. As you can see, for low n values, particulary for $D = 4.5$, the imaginary contribution to the E is very small.

One can ask what the contribution of the resonance to the density of states is. The answer to this question is given by (23).

For a single resonance with complex energy $E = E_r - iE_i$ we obtain

$$d_R(E) = -\frac{1}{\pi} Im(\frac{1}{E - E_r + iE_i}) = -\frac{1}{\pi} \frac{E_i}{(E - E_r)^2 + E_i^2}$$

which is a Lorentzian function centred at $E = E_r$ with half width at half maximum (HWHM) $\Delta = E_i$.

If E_i is small, then the width of this Lorentzian function will be small and dificult to see in the density of states.In figure 6 we plot the density of

n	E_r	E_i
0	0.496044538	1.341423967 x 10^{-13}
1	1.46237772	2.237865526 x 10^{-10}
2	2.388447199	1.464555306 x 10^{-7}
3	3,263080971	4.792204196 x 10^{-5}
4	4,062232185	0.007422203

Figure 5: Values of the real (E_r) and the imaginary (E_i) part of the Energy (E) for each n in the case $D = 4.5$.

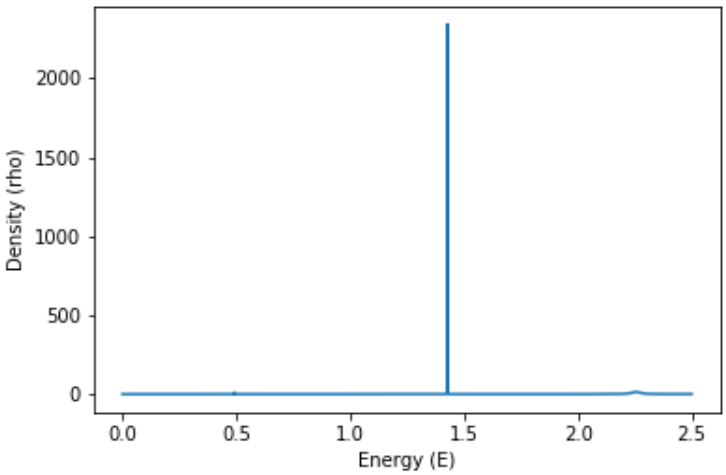

Figure 6: Density of states for D=2.5

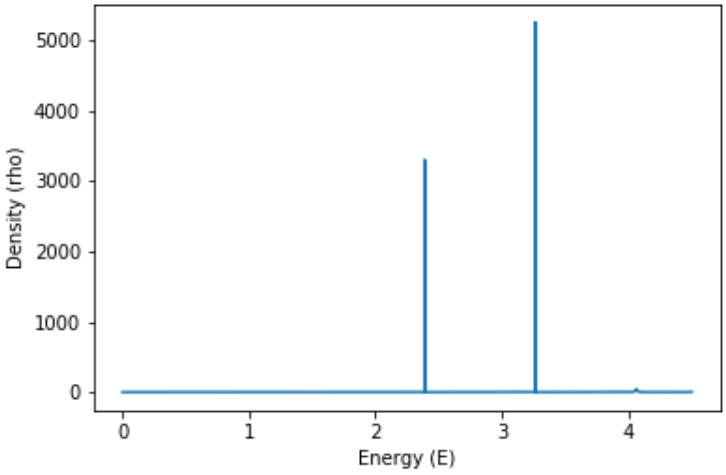

Figure 7: Density of states for D=4.5

states obteined from equation (28). In this figure, we can hardly see the first resonace ($n = 0$) at $E_r \simeq 0.49723$. However, we can clearly see the second peak at $E_r \simeq 1,42667$ and the third, which is wider because of its greater E_i value, at $E_r \simeq 2,25679$ (see figure 4).

In figure 7 we plot the same density but for $D = 4.5$,we have used 50000 points from $E = 0$ to $E = D = 4.5$. The first two peaks are so narrow that we can not see them with our resoultion. In order not to miss a resonance, we can plot the density of states in the neighbourhood of a resonance. For instance, figure 8 shows the density of states for the third resonace to $D = 2.5$, which corresponds to the $E_r \simeq 2,25679$. In this plot, we express the density of states as a function of x, an scaled magnitude from which the energy E is obtained as

$$E = -xE_i + E_r.$$

Notice that the form of the peak corresponds to the Lorentzian function of the $d_R(E)$

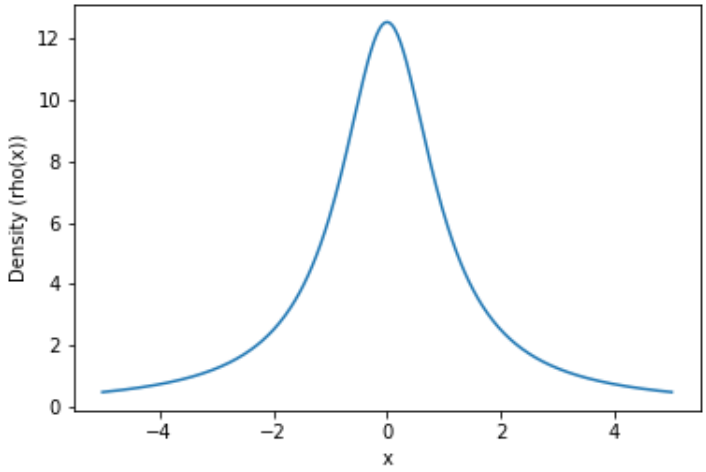

Figure 8: Third peak for D=2.5 as a function of the scaled magnitude x, centred at $x = 0$ and with Δ(HWHM)=1.

Conclusions

-We have introduced the WKB approximation as a fundamental aprroximation of semi-classical mechanics, and found its analitical solutions in the case of 1d problems, which leads to the Bohr-Sommerfield quantization condition WKB solution.

-We have also presented the semiclassical WKB solution to the time dependent Schrödinger equation for a particle in the precense of a potential in the multidimesional configuration space.

-From the previous semi-classical solution we have obtained the semi-classical Van-Vleck propagator.

-From the Van-Vleck expression by Laplace transformand stationary phase aproximation (Apendix I) we have obtained the semi-classical expresion for the Green function.

-Based on this expression we have obtained the Gutzwiller trace formula, which gives the trace of the Green function as an addition of the contributions of all the classical periodic orbits of the system. An additional step leads straightforwardly to the semi-classical density of states.

-We have applied this formalism to the case of 1d particle in a cubic potential and we have obtained, for this system an analythical expression for the complex energy (E) of the quantum resonances and for the density of states. An important result is that we have required the use of complex trayectories to account for the tunelling phenomena that are relevant in this system.

Apendix I: Method of stationary face

We need to evaluate integrals of the type

$$I = \int dx A(x) e^{is\Phi(x)}, \qquad x, \Phi(x) \in \Re,$$

where s is a real parameter. Here s will always be assumed large.

In this case, the phase oscillates fastly and "averages to zero" everywhere except at the *extremal points* $\Phi'(x_0) = 0$. Consider first the case of a 1-dimensional integral, and expand $\Phi(x_0 + \delta x)$ around x_0 to the second order in δx,

$$I = \int dx A(x) e^{is(\Phi(x_0) + \frac{1}{2}\Phi''(x_0)\delta x^2 + ...)}.$$

If near x_0 ther amplitude A(x) changes slowly over many oscilations of the exponential function, we obtain

$$I \approx A(x_0) e^{is\Phi(x_0)} \int dx e^{\frac{1}{2}is\Phi''(x_0)(x-x_0)^2}.$$

The *Fresnel integral formula*

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} dx e^{-\frac{x^2}{2ia}} = \sqrt{ia} = |a|^{\frac{1}{2}} e^{\frac{i\pi}{4}\frac{a}{|a|}},$$

takes us to

$$I \approx A(x_0) |\frac{2\pi}{s\Phi''(x_0)}|^{\frac{1}{2}} e^{is\Phi(x_0) \pm i\frac{\pi}{4}}.$$

Now, we will generalize this method for d dimensions, considering stationary phase point fulfilling the condition

$$\frac{d}{dx_i}\Phi(x) \mid_{x=x_0} = 0 \quad \forall i = 1, ..., d,$$

and the second order expantion of the phase involves the symmetric matrix

$$D_{ij}(x_0) = \frac{\partial^2}{\partial x_i \partial x_j}\Phi(x) \mid_{x=x_0} .$$

In a suitable coordinate system (which diagonalize D), we could approximate the d-dimentional integral by d 1-dimentional Fresnel integrals, obtaining

$$I \approx \sum_{x_0} (2\pi i/s)^{d/2} |\det D(x_0)|^{-1/2} A(x_0)\ e^{i(s\Phi(x_0) - \frac{\pi}{2}m(x_0))},$$

where the sum runs over all stationary phase points x_0 of $\Phi(x)$ and $m(x_0)$ counts the number of negatives eigenvalues of $D(x_0)$, which can not have zero eigenvalues.

References

[1]: L.Landau, and E.Lifshitz, (1982). *Quantum Mechanics: Non-Relativistic Theory. Vol. 3.* Barcelona: Reverté.
[2]: P. Cvitanovic, R. Artuso, R. Mainieri, G. Tanner and G. Vattay (2016). *Chaos: Classical and Quantum.* Niels Bohr Institute, Cophenguen
[3]: C. Cohen-Tannoudji, B. Diu and F. Laloe (1977). *Quantum Mechanics Vol.2.* Wiley
[4]: E.Martín-Fierro (2004). *Los estados coherentes en la descripción semiclásica de la mecánica cuántica.* ULL Ph.D. Thesis
[5]: I.S. Gradshteyn, I.M. Ryzhik, Y.V. Tseytlin (2015) *Table of Integrals,Series and Products* (pp.314). Academic Press