A Brief Survey of Periodic Orbit Theory for Real and Complex Energies

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I. INTRODUCTION

When we were first taught quantum mechanics, we learned about Bohr-Sommerfield quantization conditions. They related the classical motion of the electron with its quantum nature. From those conditions, the electron's circular orbits around the nucleus in the Coulomb potential were related to its quantum energy levels. Although that theory had some inconsistencies, it gave the exact energy levels for the hydrogen atom. But we were not told that currently there exists a tool based in classical orbits that allows us to find insight into quantum mechanical problems without having to solve Schrödinger's equations, or that by semi-classical approximations we can find the approximate energy spectrum without having to find the eigenfunctions of the Hamiltonian.

This theory is known as periodic orbit theory. In periodic orbit theory, we study the classical dynamics of the system and by finding closed orbits in phase space, we are able to give approximate information on the quantum energy levels. By periodic orbits, we mean orbits that have the same position and momentum a certain time later. In some cases, as the Bohr model did, periodic orbit theory gives the exact solution. In 1970, Martin Gutzwiller found an expression for the energy density function as an expansion in periodic orbits in term of classical properties of the cycles such as period and action among others. As he puts it in his paper "Energy Spectrum According to Classical Mechanics", *"[...] it is shown that only periodic orbits make a contribution to the spectrum. This result [...] may yield the first real generalization of the Bohr-Sommerfeld conditions."*[1] The cycle expansion can be expressed as Riemann zeta functions or spectral determinants which have an exponential or superexponential convergence, being numerically favorable because some terms can give a good approximation.
We can use periodic orbit theory to study quantum dynamics in bounded systems as well as unbounded. Balian and Bloch in 1974 in their paper "Solution to the Schrodinger Equation in terms of Classical Paths" generalized it to be

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used with complex energies so that tunneling and scattering could also be studied [4].

When trying to solve quantum mechanical problems with periodic orbit theory we perform some approximations on the basis that $\hbar$ is small. Predrag Cvitanvić explains it well in his webbook: *"Semiclassical approximations to quantum mechanics are valid in the regime where the de Broglie wavelength $\lambda \sim \hbar/p$ of a particle with momentum p is much shorter than the length scales across which the potential of the system changes significantly. In the short wavelength approximation the particle is a point-like object bouncing off potential walls the same way it does in classical mechanics. The real novelty of quantum mechanics is the interference of the point-like particle with other versions of itself travelling along different classical trajectories, a feat impossible in classical mechanics."*[7]

One dimensional quantum tunneling is a well studied effect, with the aid of the WKB method, we are able to construct the wave functions inside potential wells and calculate the transmission and reflection coefficients, under the assumption that the potential is a slowly varying function. But higher dimension tunneling is still an open problem. Even numerically there are problems that are hard to address because of the precision required. A problem that would be very interesting to study would be tunneling in n-dimensions. One way to approach it would periodic orbit theory. This a very powerful method because by using local information about the system such as periodic orbits, we can obtain global information such as transition rates. We will see that the shorter orbits contribute the most, so by finding a fair amount of short orbits we can get a good approximation to the energy density.

In this report, I will review briefly periodic orbit theory and how it can be used to study a problem such as two-dimensional quantum tunneling.

II. REVIEW OF PERIODIC ORBIT THEORY

To find the expression that relates the energy density in terms of periodic orbits, we can start with Schrödinger's equation

$$i\hbar\frac{\partial\psi}{\partial t} = H\psi. \tag{1}$$

where H is generally $H = -\frac{\hbar^2}{2m}\Delta_q + U(q)$. For a bounded system, where the particle cannot escape to infinity, we can express the wave function as a linear superposition of stationary states $\phi(q)$.

$$\psi(q,t) = \sum_n c_n\phi(q)e^{-iE_nt/\hbar} \tag{2}$$

The time evolution of the wave function in terms of the propagator is

$$K(q'',q',t) = \sum_n \phi^*(q')\phi(q'')e^{-iE_nt/\hbar} \tag{3}$$

such that

$$\psi(q',t) = \int \psi(q',0)K(q'',q',t)dq'' \tag{4}$$

where $\psi(q',t)$ is the time evolution of the wave function written in terms of the initial wave function $\psi(q',0)$. Taking the complex time Fourier transform of the propagator

$$G(q'',q',E+i\gamma) = \frac{1}{i\hbar}\int_0^\infty \sum_n \phi^*(q')\phi(q'')e^{-iE_nt/\hbar}e^{i(E+i\gamma)t/\hbar}dt \tag{5}$$

where γ is a positive number assuring the convergence of the integral. *"The Green's function $G(q'',q',E)$ is simply the probability amplitude for the particle to end up at the position q'' if it is known to have started at the position q' and was propagating with energy E"* [1]. The exact Green's function is a complicated function to work with because it diverges at each energy state. It is sufficient to know the Green's function smoothed over energy, such smoothing amounts to replacing the energy in the Green's function by the complex value $E+i\gamma$, where γ is the smoothing width. [2] After integrating over time we obtain

$$G(q'',q',E+i\gamma) = \sum_n \frac{\phi^*(q')\phi(q'')}{E-E_n+i\gamma}. \tag{6}$$

After integrating over the 3-dimensional space, for $q''=q'=q$

$$\int d^3q\ G(q,q,E+i\gamma) = \sum_n \frac{1}{E-E_n+i\gamma} \tag{7}$$

Since the delta function can be expressed as

$$\delta(E-E_n) = \lim_{\gamma\to 0^+} \mathrm{Im}\,\frac{1}{E-E_n+i\gamma} \tag{8}$$

we can write the energy density in terms of the Green's function

$$d(E) = \sum_n \delta(E-E_n) = -\frac{1}{\pi}\mathrm{Im}\int d^3q\ G(q,q,E) \tag{9}$$

which means that finding the density of energy levels is related to the zeros of the trace of the Green's function.

In 1970, Gutzwiller presented an approximate expression for the Green's function: *"In the classical limit, $G(q'',q',E)$ is approximated by*

$$G(q'',q',E) = -\frac{1}{2\pi\hbar^2}\sum_{classical\ orbits}|D_s|^{\frac{1}{2}}\exp\ i\left[\frac{S(q,q',E)}{\hbar} - phases\right] \tag{10}$$

where

$$S(q'',q',E) = \int_{q'}^{q''} pdq \tag{11}$$

and D_s is the 4-by-4 determinant of second derivatives

$$D_s = \begin{vmatrix} \frac{\delta^2 S}{\delta q''\delta q'} & \frac{\delta^2 S}{\delta q''\delta E} \\ \frac{\delta^2 S}{\delta E\delta q'} & \frac{\delta^2 S}{\delta^2 E} \end{vmatrix} \tag{12}$$

where the phases are given by $\pi/2$ multiplied by the number of conjugate times along the trajectory" [1]. D_s is a 4-by-4 determinant because q' and q'' are both 3-dimensional vectors.

One point Gutzwiller addressed in his 1970 paper [1] was whether if we replaced the exact Green's function by the approximate one, would the spectrum have the same δ-function singularity for each energy eigenvalue or not. As he shows in that paper, sometimes the spectrum structure is conserved and in others it is not. Gutzwiller compares the density of states for the particle in the box in 1, 2 and 3 dimensions using both the exact and approximate Green's function. For the 1 and 3 dimensional problems the exact and approximate Green's functions coincide, as well as the energy density. In two-dimensions, they do not coincide but the approximate energy density has the required poles. In between the poles, the energy density is an oscillating function whose total energy integral is zero. Although the approximate density of states does not vanish between the δ-function singularities, its integral vanishes. The approximate Green's function does not introduce any "new states" with a continuous distribution in addition to the discrete states [1] From the approximate Green's function, we can deduce what conditions do the orbits have to satisfy to contribute the most. Since $q'' = q' = q$, the magnitude of the momenta at the beginning and at the end of the orbit are equal $|p''| = |p'| = \sqrt{2m(E-V)}$. There are two options, either the initial and final momenta are parallel or antiparallel. To know which contributes the most we can look at the integral of the action. Through the integration over q, the action changes, with a rate given by

$$\frac{\delta S(q,q,E)}{\delta q} = p'' - p' \tag{13}$$

The phase in the approximate Green's function is constant if $p'' = p'$, otherwise it would oscillate and average less than if it had a constant value. For the same inital and final momentum, the trajectory closes smoothly on itself and is a periodic orbit. For the opposite case $|p''| = -|p'|$, the trajectory closes but is not smooth since its direction changes abruptly. In the classical approximation, $\hbar \to 0$, the contribution to the Green's function from the non-smooth trajectories is negligible compared to the contribution from periodic ortbits. The energy spectrum depends solely on periodic orbits, although the wave functions depends both on smooth and nonsmooth trajectories.[1] The trace of the Green's function in terms of properties of periodic orbits is widely known as the Gutzwiller trace formula.

$$TrG(E) = TrG_0(E) + \frac{1}{i\hbar}\sum_{p=0}^{\infty} T_p \sum_{r=0}^{\infty} \frac{1}{|det(1-J_p^r)|^{1/2}} e^{ir(S_p/\hbar - \mu(E)\pi/2)} \tag{14}$$

where p refers to prime periodic orbits and r denotes repetitions of the prime orbits. Prime orbits are periodic orbits that cannot be decomposed into smaller periodic segments. T_p is the period of the prime orbit, J_p^r is the stability matrix, and μ is the Maslov index and counts the amount of times the amplitude of the wave function vanishes over the prime orbit. G_0 is the contribution from the orbits of infinitesimal duration and can be shown that its trace is the average value of the density of energy levels $\overline{d(E)}$. So the second term, which depends on the periodic orbits, is responsible for the oscillations around an energy E.

We can write the density of oscillations as

$$d(E) = \overline{d(E)} + \frac{1}{\pi\hbar}\sum_{p,r} T_p \frac{1}{|det(1-J_p^r)|^{1/2}} \cos r(S_p/\hbar - \mu(E)\pi/2) \tag{15}$$

We could find the zeros of this function in order to find $d(E)$, but the series has a convergence problem. It is better to employ other expressions, such as the spectral determinant or the Riemann zeta function. Gutzwiller trace formula can be transformed into the spectral determinant $\Delta(E)$

$$\Delta(E) = e^{i\pi N(E)} \exp\left(-\sum_{p,r} \frac{e^{ir(S_p/\hbar - \mu_p\pi/2)}}{r|det(1-M_p^r)|^{1/2}}\right) \tag{16}$$

where N(E) is the number of energy states below E. The spectral determinant can be written in terms of the Riemann zeta function as

$$\Delta(E) = \prod_m \frac{1}{\eta_m(E)} \tag{17}$$

with

$$\frac{1}{\eta_m(E)} = \prod_p \left(1 - \frac{e^{ir(S_p/\hbar - \mu(E)\pi/2)}}{|\Lambda_p|^{1/2}{\Lambda_p}^m}\right) \tag{18}$$

We can write the Riemann zeta function as

$$\frac{1}{\eta_m} = \prod (1 - t_p^m) \tag{19}$$

where

$$t_p^m = -\frac{e^{ir(S_p/\hbar - \mu(E)\pi/2)}}{|\Lambda_p|^{1/2}\Lambda_p^m} \tag{20}$$

and p denotes the sequence or *name* describing the prime orbit. Now the energy levels are related to the zeros of the Riemann zeta function. Although the product is a nice compact expression, the factors of the product are not the zeros we are looking for and the convergence of this product is not evident. It is prefereable to expand the product and regroup the terms in a convenient manner. In order to do this, we need to be able to organize them. One tool used to classify periodic orbits is symbolic dynamics. This can be seen as a way to give a unique name to each periodic orbit. Each letter of the name is a symbol given to the particle when it does a particular thing.

Assuming that one can construct a suitable symbolic dynamics so that one can order the periodic orbits, we can regroup them according to the number of symbols in their *name* After developing the product, we obtain

$$\frac{1}{\eta_m} = 1 - \sum_{p_1+\cdots+p_k}{}' t_{p_1+\cdots+p_k} \tag{21}$$

with

$$t_{p_1+\cdots+p_k} = (-1)^{k+1} t_{p_1} \cdots t_{p_k} \tag{22}$$

and where the primed sum means the summation is to be taken over prime orbits and their combinations, without repetitions. For example, for a binary symbolic dynamics the series might look like

$$\begin{aligned} \frac{1}{\eta} &= 1 - t_0 - t_1 - t_{01} - t_{001} - t_{0001} - t_{0011} - t_{0111} - \cdots - t_{0+1} - \\ & t_{0+01} - t_{01+1} - t_{0+001} - t_{0+011} - t_{0001+1} - t_{011+1} + \cdots - t_{0+01+1} - \cdots \end{aligned} \tag{23}$$

It is commonly refered to as cycle expansion. They can be regrouped according to orbit length, as

$$\begin{aligned} \frac{1}{\eta} &= 1 - t_0 - t_1 - [(t_{01} - t_1 t_0)] - [(t_{001} - t_0 t_{01}) + (t_{011} - t_0 t_1)] - \\ & [(t_{0001} - t_0 t_{001}) + (t_{0111} - t_{011} t_1) + (t_{0011} - t_{001} t_1 - t_0 t_{011} + t_0 t_{01} t_1)] - \cdots \end{aligned} \tag{24}$$

It has the form $1 - \sum t_f - \sum c_n$ where $\sum t_f$ is the fundamental contribution and $\sum c_n$ is the correction to curvature. Here 0 and 1 are the fundamental cycles, with which you can approximate the other longer cycles. The terms that correspond to longer orbits are partially cancelled by combinations of shorter orbits. It can be shown that the terms in square brackets decrease exponentially fast. The fast convergence of this series is the reason why Riemann's zeta functions and spectral determinants are of much interest. The orbits with the greatest contribution are those with the shortest symbolic name because they usually are the most stable and have the least action. Numerically this is very important because we only need to find the shortest cycles to obtain a good precision, but on the other hand if one misses one of the small cycles then that determines the precision of the calculation regardless of how many additional orbits one has. To find the energy level density one has to find the most periodic orbits of the system and compute its period, action, Maslov index and stability matrix.

The fast convergence of the spectral determinant and the Riemann zeta function are of much interest, as Predrag Cvitanovic says in his book *"[...] finite order estimates of zeros of dynamical zeta functions and spectral determinants converge exponentially or superexponentially to the exact values, and so the cycle expansions ... represent a true perturbative approach to chaotic dynamics"* [7]

The trace formula mentioned before was only valid for real orbits, but there is a similar expression for complex orbits in classically forbidden regions presented by Balian and Bloch in ref. [4]

Starts by finding a semiclassical solution to Green's function for the Schrödinger's equation

$$[-\hbar^2\Delta + V(r) - E]G(r, r', E) = \delta(r - r') \tag{25}$$

with units $m = 1/2$ and we assume the solution has the form

$$G \approx G_0 = Ae^{iS/\hbar} \tag{26}$$

After we substitute this ansatz, we obtain an equation for the real part and another one for the complex part. If we assume A to be a smooth function, we can neglect the $\hbar^2$ term. One of the equations is the Hamilton-Jacobi equation $(\nabla S)^2 = E - V(r)$ and the other one relates the phase and the amplitude $\nabla.(A^2\nabla S)$. From the first one, we get the usual action integral

$$S = \int_{r'}^{r} \sqrt{E - V(r)}ds \tag{27}$$

where the action integral is taken along the classical trajectory going from r to r', which minimizes the integral. For real energies, the Green's function is divergent at every energy level so is best to give the energy a finite complex part to avoid divergences. For complex energies, $z = E + i\gamma$, the action is complex and must have a positive complex part so it goes to infinity at infinity and G_0 vanishes. For a region where $r - r'$ is small and $V(r)$ can be assumed constant, an approximate solution to S would be $S = |r - r'|\sqrt{z - V}$. If we want to construct a better solution we can change the constant V for a function $U(r, r', z)$ and substitute $S(U)$ into $(\nabla S(U))^2 = z - V(r)$ and get an equation for U in terms of r,r' and z. For r close to r', this equation can be expanded in powers of $\rho = |r - r'|$. The first few terms in the expansion of $U(r, r', z)$ are

$$U(R, \rho, z) = V(R) + \frac{1}{48}\left[2(\rho \cdot \nabla_R)^2 V(R) + \frac{\rho^2}{z - V(R)}(\nabla_R V)^2\right] + O(\rho^4) \tag{28}$$

where $R = (r + r')/2$ [**?**]. Since there are no odd terms of $|r - r'|$, the symmetry property of S is satisfied. The amplitude of G_0 can be found from geometric considerations as a function only of S and was calculated by Balian and

Bloch in 1970:

$$A^2(r,r',E) = \frac{-1}{(4\pi\hbar^2)^2 \frac{\delta S}{\delta r_c{}'} \frac{\delta S}{\delta r_\gamma}} \begin{vmatrix} \frac{\partial^2 S}{\partial r_a{}' \partial r_\alpha} & \frac{\partial^2 S}{\partial r_a{}' \partial r_\beta} \\ \frac{\partial^2 S}{\partial r_b{}' \partial r_\alpha} & \frac{\partial^2 S}{\partial r_b{}' \partial r_\beta} \end{vmatrix} \tag{29}$$

where a, b, c, and α, β, γ are cyclic permutations of the coordinates. These expression is valid for real and complex energies [**?**]. So once the action is found from the Hamilton Jacobi equation, the amplitude of the Green's function G_0 can also be calculated. From the action S found in terms of $U(r,r',E)$, the leading term in the Green's function expansion is

$$G_0 = \frac{1}{4\pi\hbar^2} \frac{e^{\frac{i|r-r'|}{\hbar}\sqrt{z-V(r)}}}{|r-r'|}. \tag{30}$$

For real energies, we have a set of classical trajectories for each initial position and energy, which usually have a caustic that divides the space into allowed and forbidden regions, also known as the classical and non-classical regions. In the non-classical region, the action is imaginary and the caustic is defined by its singularities.

Since the exact Green's function diverges at every energy level, we needed to introduce a finite imaginary part to the energy $z = E + i\gamma$, mentioned earlier. When we deal with complex energies, there is no longer a definite distinction between the classical and non-clasical regions. For G_0 to decay at infinity the imaginary part of the action must diverge at infinity. The approximation $G \approx G_0$ defines an outgoing wave initiating at r', the reflected waves appear as corrections to the semiclassical approximation. If now we assume G to be $G \approx G_0 + G_1$, and substitute it into the Schrödinger's equation, we get

$$[-\hbar^2\Delta + V(r) - z]G_1(r,r') = \Gamma(r,r') \tag{31}$$

where $\Gamma(r,r') = \delta(r-r') + [\hbar^2\Delta - V(r) + z]G_0(r,r')$ with has a solution for G_1 which may be written as

$$G_1(r,r') = \int d^3r'' G(r,r'')\Gamma(r'',r'). \tag{32}$$

So an expression for the Green function is

$$G(r,r') = G_0(r,r') + \int d^3r'' G(r,r'')\Gamma(r'',r') \tag{33}$$

and by iteration, we get

$$G(r,r') = G_0(r,r') + = \int d^3r'' G(r,r'')\Gamma(r'',r') + = \int d^3r'' d^3r''' G(r,r'')\Gamma(r'',r''')\Gamma(r''',r') + \cdots \tag{34}$$

The second term describes a wave going from r' to r'' near the caustic, and from there to r. The following terms describe multiple reflections of the wave on the caustic. With the approximate expression for G_0 we can find an expression for Γ for r not equal to r':

$$\Gamma(r,r') = \hbar^2\Delta A(r,r')e^{iS/\hbar} \tag{35}$$

The integrations in $G(r,r')$ are over points on the caustic, which separate the classical and non-classical regions. *"Dominant contributions will come from the neighbourhood of the point a where the phase $S(ra) + S(ar')$ is stationary. This point a is where a classical trajectory going from r' to r touches the caustic. Thus, we see that* *multiple reflection of the waves on the caustic yields the various contributions to the Green's function corresponding to the various trajectories going from r' to r. The interference between these various contributions produces oscillations in G, which correspond to shell effects."* [2] Shells are regions where there is a high density of energy levels.

After having an approximate expression for the Green function we are able to calculate the density of particles having energy E

$$n(r,E) = \frac{1}{\pi}\mathrm{Im}\, G(r,r',E) \tag{36}$$

The first term gives the Thomas-Fermi approximation

$$n^{(0)}(r,E) = \frac{1}{\pi}\mathrm{Im}\, G_0(r,r,E) = \frac{1}{4\pi^2\hbar^2} \tag{37}$$

which is related to trajectories of length zero. The other terms are oscillatory functions of the energy. At high energies, the action is large compared to $\hbar$ and the oscillations contribute to the energy density function. If the complex part of E is large then the decaying exponentials wipe out the oscillations, leaving only the leading term. Thus to each set of closed classical trajectories there is associated an oscillatory term in the energy density. If the system has some type of symmetry then it gives rise to degenerate paths, meaning a set of paths all having the same action.

Since Γ depends on the action, which is imaginary, there is some damping due to γ, so the most important contributions are associated with the shortest classical closed trajectories. Since the energy density to first approximation goes as e^{iKL}, where $K = \sqrt{E-V(r)}$ and L is the length of the trajectory. If we allow complex orbits in forbidden regions, then $K = K_R + iK_I$ and $L = L_R + iL_I$ and they have an additional damping factor given by $e^{K_R L_I}$, so complex paths can contribute if they are sufficiently short. For real energies, calculating the energy density levels through this formalism is quite straight forward, because the Green's function can be found in terms of the action, which can be computed along classical trajectories by integrating Hamilton's equations, but for complex energies the S has no variational property connecting it to paths in the real three dimensional space, and should in principle be determined by solving the complex Hamilton-Jacobi quations, which is nearly as complicated as solving the original Schrödinger equation. For analitycal potentials, we can find a relation between the Green's function and classical paths.

We can start by writing the Green's function expansion in terms of the amplitude A and the phase S, remembering that Γ goes as $\Delta A \exp(\frac{iS}{\hbar})$

$$G(r,r') = \frac{1}{\hbar^2}\sum_{p=0}^{\infty}\int d^3r_1\cdots d^3r_p A(r,r_p)\Delta A(r_p,r_{p-1})\cdots\Delta A(r_1,r')\exp\left[\frac{1}{\hbar}[S(r,r_p)+S(r_p,r_{p-1})+\cdots+S(r_1,r')]\right] \tag{38}$$

Using the Bromwich integral or inverse Laplace transform

$$\exp(at) = \frac{1}{2\pi i}\int_{\alpha-i\infty}^{\alpha+i\infty} e^{st}\frac{1}{s-a}ds \tag{39}$$

where α is a vertical contour in the complex plane chosen such that all singularities of $1/(s-a)$ lie to the left of it, we can write the exponential in $G(r,r')$ as

$$\frac{1}{2\pi i}\int_{-\infty}^{\infty} ds\; e^{is\hbar}\frac{1}{s-[S(r,r_p)+S(r_p,r_{p-1})+\cdots+S(r_1,r')]} \tag{40}$$

Now we can write Green's function as

$$G(r,r') = \frac{1}{2\pi i\hbar^2}\int_{-\infty}^{\infty} ds\ e^{is/\hbar}\Omega(r,r',s) \tag{41}$$

where

$$\Omega(r,r',s,z) = \sum_{p=0}^{\infty}\int d^3r_1\cdots d^3r_p \frac{A(r,r_p)\Delta A(r_p,r_{p-1}\cdots)\Delta A(r_1,r'))}{S(r,r_p)+S(r_p,r_{p-1})+\cdots+S(r_1,r')} \tag{42}$$

Ω depends only on classical complex paths joining the sucessive points r', r_1,... ,r_p and does not contain $\hbar$. Ω can be seen as the Laplace transform of $i\hbar^2 G$ with respect to $1/\hbar$. The integration in the Green's function definition is over vertical contours C_α in the complex plane surrounding singularities which are branch points in general. The singularities of Ω are the stationary values of the action with respect to the integration over intermediate points in the trajectory. The integration can be rewritten in terms of the loops C_α

$$G(r,r') = \frac{1}{2\pi i\hbar^2}\sum_\alpha\int_{C_\alpha} ds\ e^{is/\hbar}\Omega(r,r',s) \tag{43}$$

The function $\Omega(r,r',s)$ is discontinuous across each branch starting at S_α and extending vertically to $i\infty$, so $G(r,r')$ can be rewritten as

$$G(r,r') = \frac{1}{2\pi i\hbar^2}\sum_\alpha e^{iS_\alpha(r,r')/\hbar}\int_0^{\infty} dt e^{-t/\hbar}\delta\Omega_\alpha(r,r',t) \tag{44}$$

where the discontinuity is given by

$$\partial\Omega_\alpha(r,r',t) = \Omega(S_\alpha+it+0)-\Omega(S_\alpha+it-0) \tag{45}$$

Since the first term in the expansion of $\Omega(r,r',s,z)$ diverges as

$$\Omega_0 = \frac{A(r,r')}{s-S(r,r')} \tag{46}$$

we can define a closed paths generating function

$$\Sigma(s,z) = \int d^3r(\Omega(r,r',s,z)-\Omega_0) \tag{47}$$

to be able to calculate the remaining terms for the energy density. This function is also discontinuous around the branch point

$$\delta\Sigma_\alpha(t) = \Sigma(S_\alpha+it+0)-\Sigma(S_\alpha+it-0) \tag{48}$$

Now the energy level density can be written as

$$\rho_\gamma(E) = \rho_\gamma^{TF}(E) = +\frac{1}{2\pi^2\hbar^2}\sum_\alpha \operatorname{Im} e^{iS_\alpha}\int_0^{\infty} dt\ e^{-t/\hbar}\delta\Sigma_\alpha(t) \tag{49}$$

where ρ_γ stands for the Thomas-Fermy approximation. If we include all the complex orbits this is an exact expression for the energy level density. It can be thought of as the trace formula for complex orbits.

This sumerizes very briefly periodic orbit theory for classical and quantum dynamics. There has been some attempts at understanding quantum tunneling with periodic orbit theory. In particular, Olivier Sigwarth, Stephen Creagh and Niall D. Whelan [5],[6] have been employing complex periodic orbits to study quantum tunneling through a barrier in a two-dimensional double well potential given by

$$V(x,y) = (x^2-1)^4 + x^2y^2 + \mu y^2. \tag{50}$$

This is a double well potential with two minima at $(x = 1, y = 0)$ and $(x = -1, y = 0)$ and a saddle point at (x=0,y=0) Studying the quantum dynamics inside this potential, has been quite complicated because the classical dynamics inside the well is chaotic and it has not been possible to define a symbolic dynamics. According to Olivier Sigwarth there are various orbits very close in space with different stabilities that are hard to differentiate with the use Poincare sections. Since the shortest complex orbits are the ones which contribute the most, regardless of not having a simbolic dynamic, he has decided to find the short orbits tunneling through the barrier. In order to do this, he finds classical orbits that arrive at the central barrier as close as possible to the x-axis. Then chooses a direct trajectory crossing the barrier through the center and continues the trajectory on the other well until the trajectory crosses again the barrier and closes the orbit.

III. COMMENTS

For the double well dynamics that we were trying to study there are still a lot of issues I haven't totally understood. The complex trajectories chosen are arbitrary because there are infinitely short paths crossing the barrier. One can choose any homoclinic orbit striking the potential to build your complex periodic orbit. Since the homoclinic orbit hits the wall an infinite amount of times you can extend a complex orbit from that point to the other well and get an infinite amount of orbits. The dynamics under the well is still under debate because you can either assume complex time and momentum, or complex position and momentum, or complex position, momentun and time, to define the dynamics under the well. Olivier Sigwarth assumed the complex trajectory below the barrier to be a straight line crossing the origin. It would be nice to check if this satisfies the complex Hamilton-Jacobi equations. Another point that needs to be clarified is the physical meaning of the Maslov index in the complex space.

There is still a lot to be understood about quantum tunneling in two dimensions and higher. Periodic orbit theory seems to be a feasible tool to study this effect because of its great results in other areas of physics and of its fast convergence in numerical implementation.

IV. BIBLIOGRAPHY

[1] Gutzwiller, M. "Energy Spectrum According to Classical Mechanics", J.Math. Phys. **11**, 1791-1805 (1970)

[2] Balian, R, and Bloch, C. "Asymptotic Evaluation of the Green's Function for Large Quantum Numbers", Ann. Phys. **63**, 592-606 (1971)

[3] Balian, R, and Bloch, C. "Distribution of Eigenfrequencies for the Wave Equation in a Finite Domain: III. Eigenfrequency Density Oscillations", Ann. Phys. **69** 76-160 (1972)

[4] Balian, R, and Bloch, C. "Solution of the Schrōdinger Equation in Terms of Classical Paths", Ann. Phys. **85** 514-545 (1974)

[5] Sigwarth, Olivier "Effet Tunnel Entre deux potentiels chaotiques", (1998)

[6] Creagh, S.C. and Whelan, N.D. "A MAtrix Element for Chaotic Tunneling Rates and Scarring Intensities", Ann. Phys. **272** 196-242 (1999)

[7] P. Cvitanović *et al.*, *Chaos: Classical and Quantum*, advanced graduate e-textbook, available online at `ChaosBook.org` (Niels Bohr Institute, Copenhagen 2003).