Unexpected Quantum Bound States In Open Potentials

Variational Tests and Classical Periodic Paths

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Abstract

We investigate the mechanisms that give rise to the two bound states at the intersection of two infinite potential well channels in two dimensions. Each channel individually has no bound states, but the intersection has two bound states. It was hypothesized by Schult [1] that the bound states arise because of the sharp corners and the possible classical bounded trajectories at the intersection. We investigate these claims and found that the sharp corners are not necessary for the existence of bound states, but the classical bounded trajectories are. We approximate the bound state energies with the Van-Vleck-Gutzwiller approximation and obtain $E_0 = 0.5E_t$ and $E_1 = 2E_t$.

Contents

1 Motivation

The present investigation is inspired by the following intriguing problem (labelled three stars!) in the Griffiths text (Problem 7.20) [2]. Consider the usual non-relativistic 2-dimensional Hamiltonian $\hat{H} = \dfrac{\hat{p}^2}{2\mu} + V(x, y)$, with the following potential

$$V(x,y) = \begin{cases} 0, & |x| < L/2 \text{ or } |y| < L/2 \\ \infty, & \text{else} \end{cases}$$

In other words, it is a 2-dimensional infinite potential well in the shape of a cross with arm channel width L.

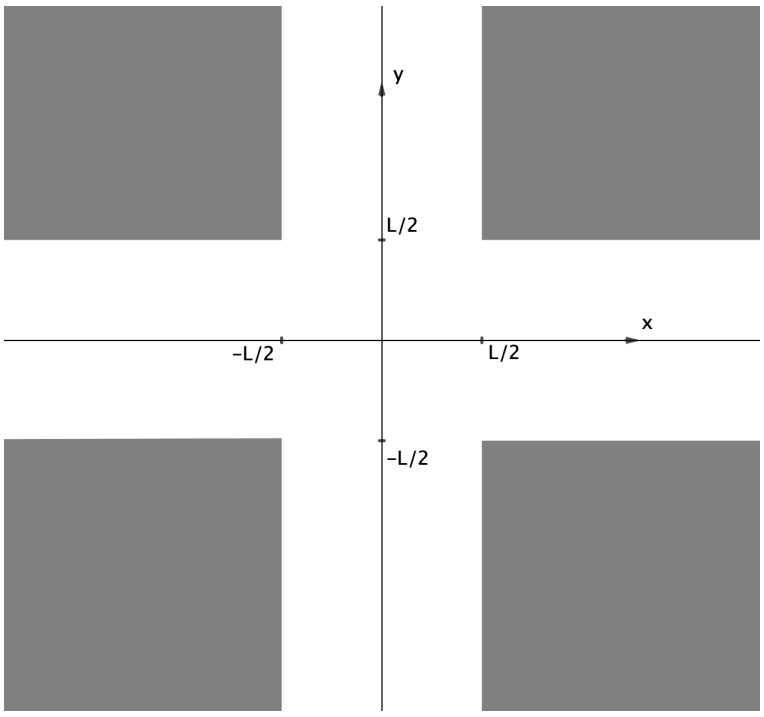

Figure 1: A 2-dimensional cross well potential. The potential is zero inside the two channels (white) and infinite outside (grey). The channels have width L.

This potential has a surprisingly remarkable feature. All states in this potential have non-negative energy, since there are no attraction sources. The potential is zero at infinity inside the arms, so the energy of all states exceed the potential at infinity. Conventional classical wisdom suggests that all states should be scattering states, propagating along on one of the four arms towards infinity. Despite of that, the ground state of this potential is actually a bound state. Griffiths playfully calls this "the reverse of tunneling": whereas tunneling refers to the idea of a classically bound particle becoming unbound due to quantum mechanics,

here a classically unbound particle becomes bound.

Like all good textbook writers, Griffiths seeks interesting problems from various papers. This particular potential is quoted from a paper modelling the intersection of two wires by Schult [1]. The original paper points out something even more remarkable: this cross-well potential has not just one, but two (!!) bound states. The ground state and the first excited state are both bound.

There is no obvious reason as to why this open-ended potential needs to have two bound states a priori. Perhaps the most convincing justification is that upon feeding this potential to a computer and solving the time independent Schrodinger equation on a 2D numerical grid, we see two states whose wave functions decay to zero at infinity. This was the argument given in the original Schult paper.

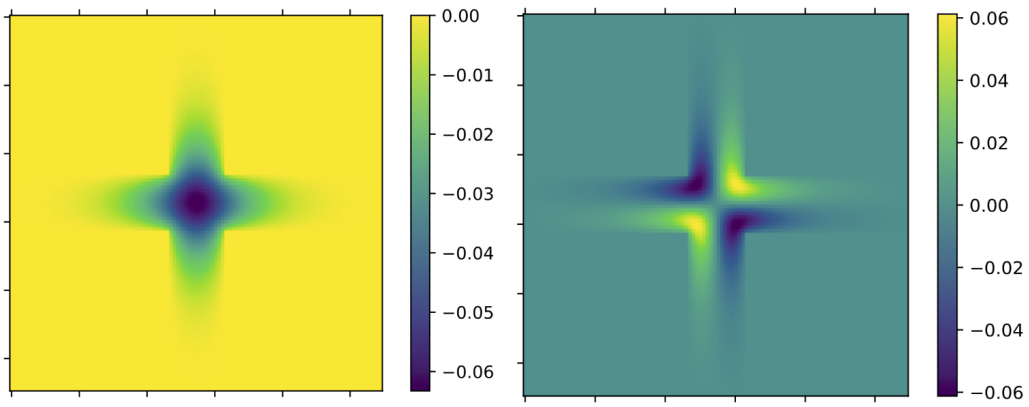

Figure 2: Solving the 2D time independent Schrodinger equation by brute force on a computer produces two bound states. The figure shows the wave functions. The ground state (left) is even about all 4 symmetry axes; the first excited state (right) is even about the two diagonal axes and odd about the x and y axes. Schult arrived at the same symmetry classes for the two bound states.

However, this explanation is infinitely unsatisfactory. In the original paper, Schult briefly discussed, in broad strokes and common-sense style arguments, two possible reasons to why this potential has bound states:

1. Because of the sharp corners in the potential.
2. Because there are classically bound trajectories in this potential.

Both of these explanations seem to have problems. On the one hand, imagine the corners are

rounded out. This is a perturbation very near the origin, and is unlikely to affect behaviors of the wave function at infinity. It is very hard to imagine that the amplitude of a state at infinity suddenly pops into existence from zero to some finite value just because infinitely far away a sharp corner became a rounded corner. On the other hand, imagine one pair of opposite arms are blocked. We are left with a single channel, i.e. free particle in one dimension and infinite well of width L in the other dimension (see figure 3). This potential also has classically bound trajectories, but it has no bound states.

Figure 3: A 2-dimensional one-channel potential well. The potential is zero inside the channel (white) and infinite outside (grey). The channel has width L. This potential has no bound states, despite the existence of classically bound orbits. A classical particle can just bounce along a fixed x infinitely and never fly off to infinity. One such bouncing orbit is shown in red.

This paper performs a more careful investigation of this potential. In particular, we carefully examine the above two claims. We will first round out the corners to test whether the bound states persist with the help of the variational principle in section 2. Then we will investigate how exactly the classically bound trajectories enter into the quantum mechanics in section 3. This will take us deep into the realms of Feynman path integral and the Van-Vleck-Gutzwiller approximation [3, 4, 5, 6, 7], which we will use to analyze the cross-well and recover the two bound states.

2 Variational Methods

2.1 Threshold energy

The first effect of quantum mechanics is that it introduces a zero-point energy in free space. While classically a particle in any potential can stay at rest with zero energy at the (either stable or unstable) equilibrium points, quantum mechanics disallows such perfectly at rest particles. Any particle prepared in a position eigenstate will necessarily disperse out in time, and infinite position precision cannot retain forever.

This is because any Hamiltonian of the form

$$\hat{H} = \frac{\hat{p}^2}{2\mu} + V(x)$$

will not commute with the position operator x, because $[\hat{p}, \hat{x}] \neq 0$ and $[V(\hat{x}), \hat{x}] = 0$. Therefore, any position eigenstate $|x\rangle$ is necessarily not an energy eigenstate. Upon time evolution, $e^{-i\hat{H}t}|x\rangle$ will not evolve as an overall phase times $|x\rangle$, and other positions will emerge as time evolution goes on.

As a quantum mechanical particle cannot stay perfectly at rest forever, it cannot have zero energy, even in free space. The ground state always has some non-zero energy, and if a particle does not have at least that amount of energy, then it cannot exist in the potential.

With this realization, let's look at our cross well potential. Consider when we are infinitely far away from the origin in one of the arms. The potential here looks like the one shown in figure 3.

The potential at infinity in one of the arms is separable as

$$V(x, y) = V_x(x) + V_y(y)$$

where

$$V_x(x) = 0, \quad V_y(y) = \begin{cases} 0, & |y| < L/2 \\ \infty, & \text{else} \end{cases}$$

Since the potential (and thus the Hamiltonian) is separable, the wave function here in one of the arms is also separable, so the total energy of a state is the simple sum of the individual energies from the two separated dimensions, i.e.

$$E = E_x + E_y$$

This is quickly justified, as the wave functions in the two dimensions decouple completely into simple tensor products for separable Hamiltonians $\hat{H} = \hat{H}_x + \hat{H}_y$:

$$\begin{aligned}(\hat{H}_x + \hat{H}_y)\,|\psi_x\rangle \otimes |\psi_y\rangle &= \hat{H}_x\,|\psi_x\rangle \otimes |\psi_y\rangle + \hat{H}_y\,|\psi_x\rangle \otimes |\psi_y\rangle \\ &= (\hat{H}_x \otimes \hat{1})\,|\psi_x\rangle \otimes |\psi_y\rangle + (\hat{1} \otimes \hat{H}_y)\,|\psi_x\rangle \otimes |\psi_y\rangle \\ &= E_x\,|\psi_x\rangle \otimes |\psi_y\rangle + E_y\,|\psi_x\rangle \otimes |\psi_y\rangle \\ &= (E_x + E_y)\,|\psi_x\rangle \otimes |\psi_y\rangle\end{aligned}$$

The two individually separated dimensions are two standard 1D problems. $V_x(x)$ is a free particle, and $V_y(y)$ is an infinite square well with width L. The energies are thus

$$E = \frac{\hbar^2}{2\mu}\left(k_x^2 + \frac{n^2\pi^2}{L^2}\right),\ n = 1, 2, 3, ...$$

Notice that this is a sum of two non-negative numbers. The smallest possible value of n is 1, so this number is never smaller than

$$E_t \equiv \frac{\hbar^2\pi^2}{2\mu L^2}$$

Therefore, at infinity in the arms, all energy eigenstates need to have energy at least this E_t, or have zero wavefunction (in which case the time-independent Schrodinger equation is trivially satisfied as $0 = 0$). If the cross-well potential has an energy eigenstate with an energy smaller than this threshold, then its wavefunction must be zero in the arms at infinity, and has to only exist in the cross near the origin. In other words, it would be a bound state.

2.2 Ground state variational principle

The fact that bound states will arise for energies lower than a threshold energy E_t prompts us to use the variational principle. The variational principle puts an upper bound on the ground state energy, and if this bound is itself smaller than E_t, then the ground state must be lower than E_t and hence is a bound state.

The variational principle is introduced in many introductory quantum mechanical textbooks [2, 8]. Let us quickly review the variational principle. For any Hamiltonian $\hat{H}$ with energy spectrum $\{E_i\}$, consider an arbitrary trail state $|\alpha\rangle$ that is normalized (that is, $\langle\alpha|\alpha\rangle = 1$). Variational principle states that the energy expectation value of this arbitrary $|\alpha\rangle$ state must be higher than the ground state energy E_{gs}. The proof of this powerful principle is

embarrassingly easy. The trick is to expand $|\alpha\rangle$ onto the energy eigenbasis, and use the fact that all energies in the spectrum are greater than or equal to the ground state energy.

$$\begin{aligned}
\langle\alpha|\hat{H}|\alpha\rangle &= \sum_i \sum_j \langle\alpha|i\rangle \langle i|\, \hat{H}\, |j\rangle \langle j|\alpha\rangle \\
&= \sum_i \sum_j \langle\alpha|i\rangle E_i \delta_{ij} \langle j|\alpha\rangle \\
&= \sum_i \langle\alpha|i\rangle E_i \langle i|\alpha\rangle \\
&\geq \sum_i \langle\alpha|i\rangle E_{gs} \langle i|\alpha\rangle \\
&= E_{gs}
\end{aligned}$$

Note that $\langle i|\, \hat{H}\, |j\rangle = E_i \delta_{ij}$ because the Hamiltonian is diagonal in the energy eigenbasis. The last equal sign is true because with E_i replaced by E_{gs}, the sum is only on $\sum_i |i\rangle \langle i|$ which reduces to identity, and $\langle\alpha|\alpha\rangle = 1$.

An important point to realize is that, because the variational principle stands on the resolution $|\alpha\rangle = \sum_i |i\rangle \langle i|\alpha\rangle$, we can cherry-pick this resolution and allow only a subset of all states to participate by designing a trail state that is orthogonal to some non-participating states, and the upper bound will be on the lowest of this participating subset. For example, in one dimension with a symmetric potential, an odd trail wavefunction will put a upper bound on the first excited state, not the ground state, because an odd trail wavefunction contains only odd states in the resolution, and the ground state is even. This point will be important when we address the first-excited state. Without any cherry-picking, this resolution is over all energy eigenstates, and the upper bound is on the absolute lowest state of the entire spectrum (i.e. ground state).

It is now time to design a trail wave function for the cross well (figure 1). Every energy eigenstate of the cross well is zero on the boundaries (i.e. the lines $x, y = \pm L/2$, except the central square), so any superposition of them will also be zero on the boundaries. Our trail wavefunction needs to have this property.

To avoid cluttering our equations with meaningless factors of 2, let's define the length factor $a \equiv L/2$. In other words the cross well potential has arm width $2a$. In this length unit the threshold energy is $E_t = \dfrac{\hbar^2\pi^2}{2\mu L^2} = \dfrac{\hbar^2\pi^2}{8\mu a^2}$.

A convenient trail wavefunction design that meets this constraint is

$$\Psi(r,\phi) = N\cos\left(\frac{\pi}{2r_0}r\right)u(-r+r_0), \quad r_0 \le \sqrt{2}a$$

where $u(r)$ is the Heaviside unit step function, and N is the to-be-determined normalization constant. It is a cosine-like dome over the origin with radius r_0, and zero outside the dome.

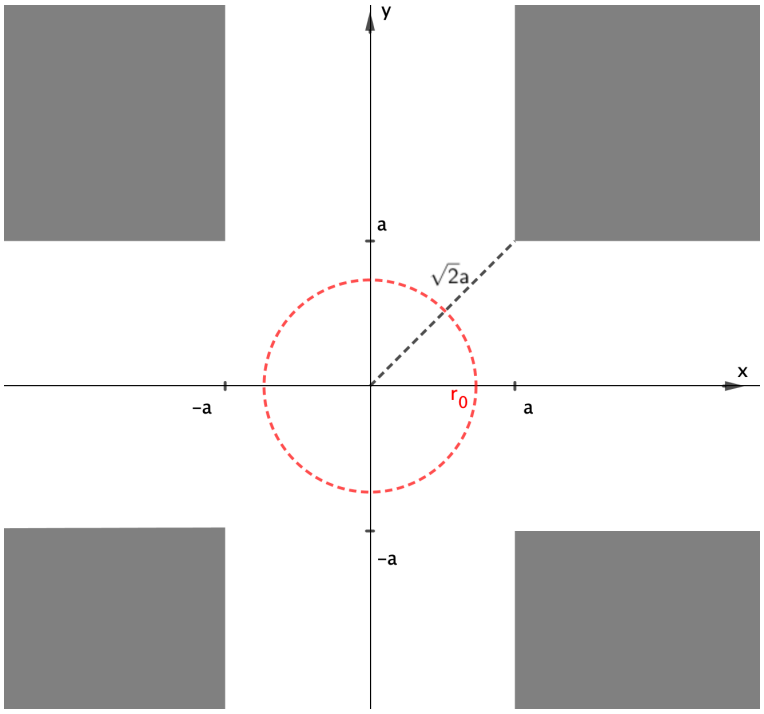

Figure 4: The domain for the variational trail wavefunction. The trail wavefunction is zero outside the red circle (since there $r > r_0$, so $-r + r_0 < 0$ and the Heaviside function is zero). The radius of the dome base is bounded above by $\sqrt{2}a$: any bigger the trail wavefunction would cut into the forbidden regions and violate the boundary constraint.

The radius of the dome base r_0 is taken to be the variational parameter.

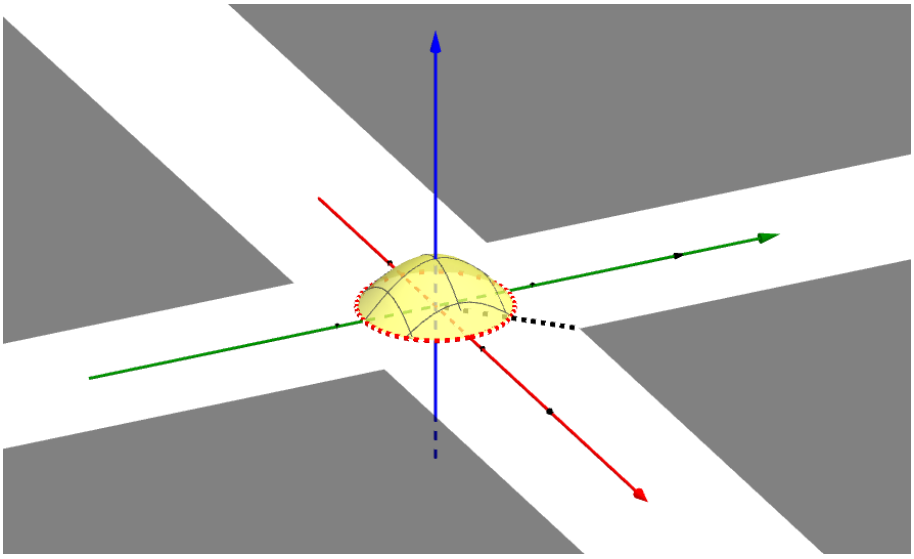

Figure 5: Inside the red circle the trail wavefunction is a dome. The cosine term $\cos(\pi r/2r_0)$ is maximum at $r = 0$ and falls to zero at $r = r_0$.

This trail wavefunction is zero on all boundary lines $x, y = \pm a$ except the middle square. It is thus a viable trail that can be constructed by superpositioning energy eigenstates. Upon running the variational principle on this trail, we will get an upper bound on the ground state energy.

The integrals involved here are rather trivial. We only sketch the outline of the computation. In particular, we demonstrate how to deal with the Heaviside step function in the integral.

The first step is to normalize the trail via

$$\int_0^\infty dr \int_0^{2\pi} d\phi \; r|\Psi|^2 = 1$$

The r in the integrand is the standard 2D polar coordinate Jacobian. For our trail this is

$$2\pi N^2 \int_0^{r_0} r \cos^2\left(\frac{\pi}{2r_0} r\right) dr = 1$$

This integral is easily done through integration by parts. We showcase this for fun here, and the more masochist reader is welcomed to check.

$$\int r \cos^2\left(\frac{\pi}{2r_0} r\right) dr = \frac{1}{4} r^2 + \frac{r_0}{2\pi} r \sin\left(\frac{\pi}{r_0} r\right) - \frac{{r_0}^2}{\pi^2} \sin^2\left(\frac{\pi}{2r_0} r\right)$$

The normalization constant is found to be

$$N = \sqrt{\frac{2\pi}{(\pi^2 - 4)\, r_0^{\,2}}}$$

We are now in a position to evaluate $\langle\Psi|\hat{H}|\Psi\rangle$. Since $\Psi(r,\phi)$ is now properly normalized, this expectation will be an upper bound for the ground state energy.

We start with

$$\hat{H}\Psi(r,\phi) = \left(-\frac{\hbar^2}{2\mu}\nabla^2 + V(r,\phi)\right)\Psi(r,\phi)$$

The potential term vanishes: inside $r = r_0 \leq \sqrt{2}a$ the potential is zero, and outside the wavefunction is zero. Also since the trail wavefunction has no angular dependence, the ϕ derivatives in the Laplacian drops away. We are left with, after plugging in the trail wavefunction,

$$\hat{H}\Psi(r,\phi) = -\frac{\hbar^2}{2\mu}N\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r}\right)\cos\left(\frac{\pi}{2r_0}r\right)u(-r+r_0)$$

The energy bound we seek is thus

$$\begin{aligned}&\langle\Psi|\hat{H}|\Psi\rangle \\ &= \int_0^\infty r dr \int_0^{2\pi} d\phi \left(N\cos\left(\frac{\pi}{2r_0}r\right)u(-r+r_0)\right)\left[-\frac{\hbar^2}{2\mu}N\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r}\right)\cos\left(\frac{\pi}{2r_0}r\right)u(-r+r_0)\right]\end{aligned}$$

This integral is very straightforward, once we use the fact that the derivative of the Heaviside step function is the Dirac Delta function. The second derivative of the Heaviside step function does not introduce any new difficulties since it can be treated with integration by parts. The detailed procedure for this integral is shown in Appendix A.

As it turns out, somewhat beautifully, this integral does not depend on the variational parameter r_0 outside of the N^2 normalization factor. It evaluates to

$$\langle\Psi|\hat{H}|\Psi\rangle = \frac{\hbar^2 N^2 \pi(\pi^2+4)}{16\mu}$$

Plugging in N, this is

$$\langle\Psi|\hat{H}|\Psi\rangle = \frac{\hbar^2}{\mu r_0^{\,2}}\frac{\pi^2(\pi^2+4)}{8(\pi^2-4)} \approx 2.9152\frac{\hbar^2}{\mu r_0^{\,2}} \geq E_{gs}$$

The energy of the trail wavefunction depends on the variational parameter trivially as a monotonic $1/{r_0}^2$. Recall that our threshold energy was $E_t = \hbar^2\pi^2/8\mu a^2$. If the variational trail wavefunction has energy lower than E_t, then the ground state energy, which is lower than the trail energy, will also be lower than the threshold, and the ground state will be bound. Thus the condition for the ground state to be bound is

$$\frac{\hbar^2}{\mu {r_0}^2}\frac{\pi^2(\pi^2+4)}{8(\pi^2-4)} < \frac{\hbar^2\pi^2}{8\mu a^2}$$

We thus have the condition for the ground state to be bound:

$$r_0 > \sqrt{\frac{\pi^2+4}{\pi^2-4}}\, a \approx 1.5372a$$

The largest r_0 for the trail dome so that it does not cut into the forbidden regions was $\sqrt{2}a \approx 1.4142a$, which is smaller than the calculated $1.5372a$. Therefore, our trail wave function does not guarantee the ground state to be a bound state. This is somewhat expected. The most important feature of our cross well is of course the four arms. However, our dome trail wavefunction does not utilize these arms at all, and just blanketly set the wavefunction in the arms to be zero, as if they were not there. The original problem in Griffiths also uses the variational principle, but it designs an exponentially-decaying tail in the arms [2]. That variational trail does guarantee a bound ground state for the cross well.

However, our results are not completely useless. Consider the cross well but with the corners rounded out by masking around the origin with a circle of radius r_0, as illustrated below in figure 6.

Our dome trail wavefunction, which is only nonzero inside the $r = r_0$ circle, is still zero on all the boundary lines. Therefore, it can be decomposed onto the energy eigenstates of this rounded cross well, all of which are zero on the boundary lines. The dome is thus a viable variational trail for this rounded cross well, and our result $r_0 > 1.5372a$ holds: the ground state of this rounded cross well is bound as long as the central circle is big enough compared to the arm widths.

Effectively we have refuted that first point made by Schult: even though the rounded potential no longer has sharp corners, bound states can still arise. In fact, our intuition suggests that as the central circle gets larger and larger, we should see more and more bound states, as eventually in the $r_0 >> 1$ limit, the arms become so tiny that the rounded potential approaches the 2D circular well which has an infinite spectrum of bound states. We now investigate what is required for the first excited state to be bound along this line of argument.

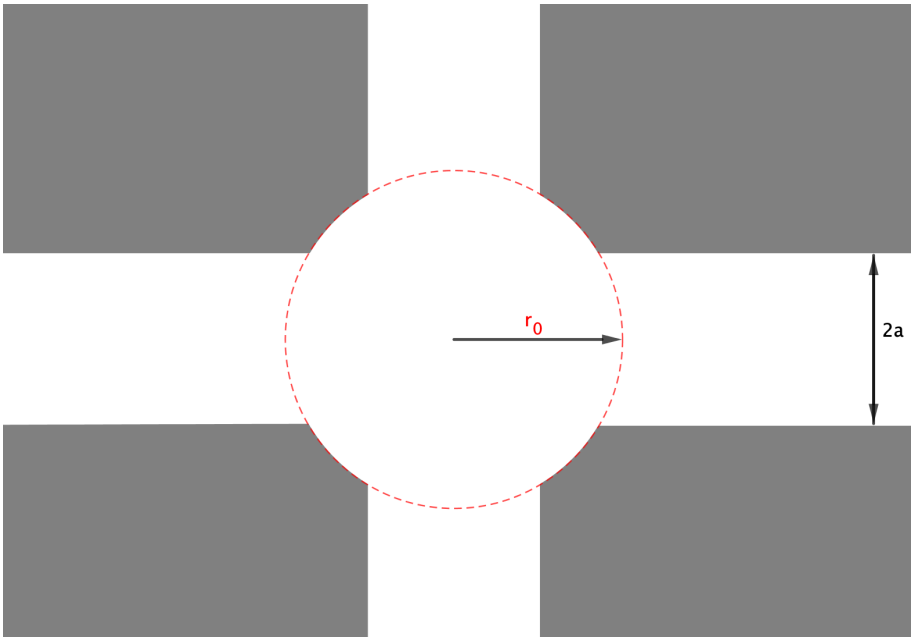

Figure 6: The cross well but the corners are rounded by a central circle of radius r_0. The ground state of this potential is bound if $r_0 > 1.5372a$.

2.3 First excited state variational principle

Recall that in the proof of the variational principle, the argument was made that the energy expectation of the trail wavefunction exceeds the energy of the lowest state contained by the trail wavefunction. If we design a trail wavefunction that is orthogonal to the ground state, then its energy expectation would give us an upper bound on the first excited state.

Although we don't know the exact ground state, all we need is that the ground state is radially symmetric, as any ϕ-dependence introduces some non-zero angular momentum and thus would not be the ground state. In other words, the ground state has no ϕ-dependence. With this in mind, we design the 1st-excited trail wavefunction to be

$$\Psi(r,\phi) = N\cos\left(\frac{\pi}{2r_0}r\right)r^2\sin(2\phi)u(-r+r_0)$$

It is essentially the ground state trail but with a oscillating angular dependence: in the 1st and 3rd quadrant the dome is positive, in the 2nd and 4th it's negative. This trail is orthogonal to the true ground state, as upon taking their inner product, the ϕ integral is $\int_0^{2\pi}\sin(2\phi)d\phi$, which is zero. We also attach a r^2 manually so that the curvature does not blow up at the origin. There is no anxiety in this step: it is our trail wavefunction after all, and we can design it however we like. Mathematically this r^2 is to cancel the $1/r^2$ in the angular derivative of the polar Laplacian.

A similar analysis as the ground state shows that for this trail, once properly normalized,

$$\langle\Psi|\hat{H}|\Psi\rangle = \frac{\hbar^2\pi^2}{8\mu {r_0}^2}\frac{\pi^2(\pi^4+30\pi^2-360)+1440}{\pi^6-30\pi^4+360\pi^2-1440} \approx 14.3546\frac{\hbar^2}{\mu {r_0}^2} \geq E_1$$

Because the first excited state is odd about the x and y center lines, its threshold energy is the first excited state energy of the 1D infinite well at infinity in one of the arms. The threshold energy for the first excited state is thus

$$E_{t,\text{odd}} = \left.\frac{\hbar^2 n^2\pi^2}{2\mu(2a)^2}\right|_{n=2} = \frac{\hbar^2\pi^2}{2\mu a^2}$$

Recall that $n = 1$ gives the threshold for the ground state (which is even about the x and y center lines).

The variational trail energy need to be smaller than the threshold for the first excited state of the cross well to be bound. Thus,

$$E_1 \leq 14.3546\frac{\hbar^2}{\mu {r_0}^2} < \frac{\hbar^2\pi^2}{2\mu a^2}$$

So the condition for the first excited state to be bound is

$$r_0 > 1.7055a$$

In other words, imagine a circular mask rounding the corners of the cross well (figure 6). We have proved, through the variational principle, that when the radius of this circular mask reaches $1.5372a$ and $1.7055a$, there will be one and two bound states, respectively. Therefore, the existence of bound states in the original cross well is not a result of the sharp corners as Schult suggested, as in a similar potential with no sharp corners, the bound states still exist.

3 Feynman Path Integrals and Classical Paths

The more impatient reader might be slightly annoyed that we are running away from the original cross well problem to discuss the circular well with a varying radius. Indeed, although we had fun applying some classroom approximation techniques in the circular well, it does not answer any questions about the original cross well and its two bound states. The circular well's radius needed to cut into the forbidden regions of the cross well a little bit for our trail wave function to guarantee bound states. Well, calm your impatience. We now turn to the overdue discussions of the cross well.

Recall that in the original investigations into the cross well, Schult argued that the two bound states arise because of the classically bound trajectories in the potential. One immediate problem arises with this argument. As discussed in the introduction section, the potential in figure 3 also has classically bound trajectories, but it has no bound states. Clearly, the roles of classically bound trajectories in quantum mechanics are more intricate. Huge amounts of work has been done on this front by Feynman [3] and Gutzwiller [4, 5, 6, 7]. We now turn to these fascinating results.

3.1 Brief review of Feynman path propagator

The role of trajectories in quantum mechanics is somewhat relegated to an aftertaste in the Schrodinger picture in a standard undergraduate curriculum. There, the focus is on the different states of energy, not on the positions of particles. It was Feynman who brought the notion of trajectories back into life in quantum mechanics. Feynman developed the path integral formulation of quantum mechanics, documented in the classic Feynman Hibbs monograph [3]. Those reader unfamiliar with the mathematical derivation of Feynman path integral is invited to consult Feynman's original monograph, or the relevant (very well-explained) sections in other more modern texts like Sakurai [8] and Zee [9]. Here we give a heuristic argument.

Consider a particle initially located at position q' at time t'. At the final time t'', the state of the particle has evolved, and upon a position measurement its position is measured to be q''. Unlike in classical mechanics, where given a definite initial coordinate (q', t') and final coordinate (q'', t'') one can be certain about the trajectory the particle took (as prescribed by the least action principle), in quantum mechanics different paths can form superposition.

For *any* path connecting q' and q'', we associate a probability amplitude. The overall am-

plitude from q' to q'' is the sum of all amplitudes of each individual path [1]. This sum is done via the following way. We discretize the time coordinate into N equal intervals $\{t_0 = t', t_1, t_2, ..., t_{N-1}, t_N = t''\}$. At each such point in time t_i, the path's location is given as q_i. The sequence of segments joining the points $\{q_0 = q', q_1, q_2, ..., q_{N-1}, q_N = q''\}$ is a path the particle could take. In this formulation, a path is simply a function of the $N-1$ spatial variable partition points q_i. A sum over all possible paths from q' to q'' is thus integrating all of these $N-1$ variable partition points over all space.

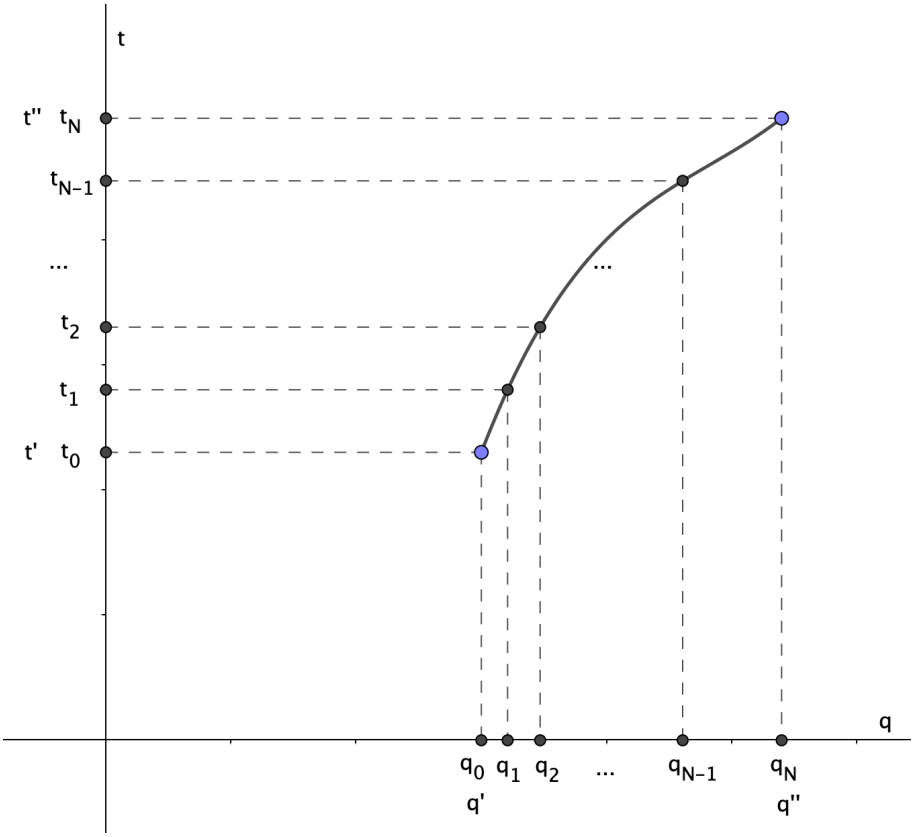

Figure 7: Discretization scheme for path integral.

The question then reduces to what the amplitude for each individual path is. It was Dirac who first realized that this amplitude for each path is given by $e^{iR/\hbar}$, where $R = \int \mathcal{L}\, dt$ is the *classical* action of the particle along the path in question, with $\mathcal{L}$ being the Lagrangian [2]. While Dirac made this observation, he never fully developed his vague hunch, and it took Feynman to finish Dirac's "mysterious remark" [8].

[1] Note that in the Schrodinger picture, this overall amplitude is nothing but $\langle q''| \exp\left(-i\hat{H}t/\hbar\right) |q'\rangle$. It is the wavefunction of the particle initially being in a position eigenstate $|q'\rangle$ and evolving for time $t = t'' - t'$.

[2] Notice how the classical action is an integral, and can be calculated in the same discretization scheme described above.

This cockamamie-looking amplitude makes perfect sense if we consider the classical limit. For classical particles, their action along a path is some 34 orders of magnitude bigger than $\hbar$. This means the phase $R/\hbar$ is a huge number. In particular, if we toggle the path a bit (by toggling one or more of the q_i's), the difference in phase will still be huge for these two nearby paths. When summing over the amplitude of all possible paths, effectively we are adding up many complex numbers with randomly distributed phases, so most of them will destructively interfere and cancel out. The only surviving paths are those whose amplitudes are the complex numbers with phases that somewhat line-up and constructively interfere. That happens precisely on paths where $\delta R = 0$, i.e. the classical trajectories where the action is stationary. On these paths, because $\delta R/\hbar = 0$, a nearby path will have roughly the same phase. The classical trajectory is therefore the only trajectory with an appreciable amplitude, and the classical particle will travel on it. Feynman, in his QED book geared towards the general public, illustrates this very nicely with the reflection of light [10].

The overall amplitude for the initial particle at (q', t') to be eventually found at (q'', t''), denoted by $\boldsymbol{K(q''t''q't')}$ and known as the **propagator**, is thus given by, gloriously,

$$K(q''t''q't') = \lim_{N\to\infty} \left(\frac{m}{2\pi i\hbar\epsilon}\right)^{\frac{nN}{2}} \int d^n q_1 \int d^n q_2 ... \int d^n q_{N-1} \exp\left(i\frac{R(q_1, q_2, .., q_{N-1})}{\hbar}\right) \quad (1)$$

where n is the dimensionality of space, and $\epsilon \equiv \dfrac{t'' - t'}{N} = t_{i+1} - t_i$ is the timestep. We make explicit of the fact that the action R is a function of the path $\{q_1, q_2, .., q_{N-1}\}$, for future convenience.

It has the structure discussed: an integral over all paths as $(N-1)$ integrals of q_i over all space, and the integrand for each path is $e^{iR/\hbar}$. The overall normalization factor is worked out by Feynman to satisfy the natural physical constraint

$$K(q''t''q't') = \int d^n q K(q''t''qt)K(qtq't') \quad (2)$$

which says that the amplitude to go from q' to q'' is the sum of amplitudes of all possible alternative paths if we imagine a "breakpoint" q in between [3]. With the normalization factor shown in equation (1), Feynman showed that this physical constraint (2) reduces to the usual Schrodinger equation [3].

Equation (1) can and should be taken as a *postulate* of quantum mechanics, as it comes from nothing but fundamental physical arguments. We will treat it as the starting point of our following discussions.

[3] In the Schrodinger picture, equation (2) is simply inserting an identity $\int |q\rangle \langle q|$ and splitting the time evolution into two time steps.

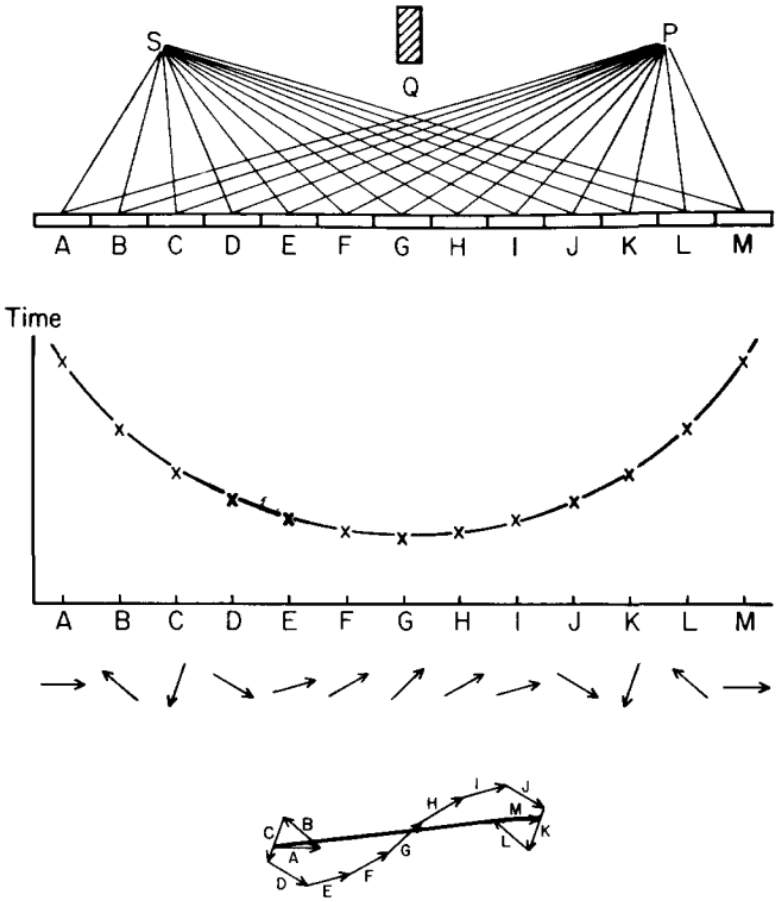

Figure 8: Feynman's illustration of the path integral in his QED book, with the reflection of light. The action for a photon along a certain path is simply the total time along the path. Outside the paths close to the symmetrical classical true path going through G, the amplitudes of most paths will destructively interfere in the phases and cancel out.

3.2 Green's function formulation

A common point of interest about the Feynman path integral formalism is how it connects to the usual Schrodinger picture, i.e. how to extract the energy levels from the propagator. This is done through the Green's function. Define the **Green's Function** $G(q'', q', E)$ as

$$G(q'', q', E) = \frac{1}{i\hbar} \int_0^\infty dt K(q''t, q'0) \exp\left(\frac{iEt}{\hbar}\right) \tag{3}$$

It is called the Green's function because it is the impulse response to the time independent Schrodinger equation, though that will not be the focus here.

Plugging in the propagator $K(q''t, q'0) = \langle q''| \exp\left(-i\hat{H}t/\hbar\right) |q'\rangle$ (see footnote 1), and noting

that the position eigenkets $|q'\rangle$ and $|q''\rangle$ don't have time dependence, we have

$$\begin{aligned} G(q'', q', E) &= \frac{1}{i\hbar} \int_0^\infty dt \, \langle q''| \exp\Big(-i(\hat{H} - E)t/\hbar\Big) |q'\rangle \\ &= \frac{1}{i\hbar} \langle q''| \left[\int_0^\infty dt \exp\Big(-i(\hat{H} - E)t/\hbar\Big) \right] |q'\rangle \\ &= \langle q''| \frac{\exp\Big(-i(\hat{H} - E)t/\hbar\Big)}{\hat{H} - E} |q'\rangle \Bigg|_{t=0}^{\infty} \end{aligned} \tag{4}$$

The $t = 0$ boundary term of the numerator is simply one since it's $\exp(0)$. The $t = \infty$ boundary term is zero. The argument goes as follows: consider E as complex. We are interested in the behavior of the numerator near the (positive) real axis. Therefore, we let E carry a small imaginary part as $E + i\epsilon$. The term is now

$$\begin{aligned} \exp\left(\frac{-i(\hat{H} - E)t}{\hbar}\right)\Bigg|_{t=\infty} &\longmapsto \exp\left(\frac{-i\hat{H}t}{\hbar}\right) \exp\left(\frac{i(E + i\epsilon)t}{\hbar}\right)\Bigg|_{t=\infty} \\ &= \exp\left(\frac{-i\hat{H}t}{\hbar}\right) \exp\left(\frac{iEt}{\hbar}\right) \exp\left(\frac{-\epsilon t}{\hbar}\right)\Bigg|_{t=\infty} \end{aligned}$$

whose modulus is zero as $E+i\epsilon$ approaches the real axis from above due to the $\exp\left(\frac{-\epsilon t}{\hbar}\right)\Big|_{t=\infty}$.

Therefore, the numerator of (4) is just $0 - 1 = -1$. We thus have

$$G(q'', q', E) = \langle q''| \frac{1}{E - \hat{H}} |q'\rangle$$

To act with the Hamiltonian, we expand $|q'\rangle$ onto the energy eigenbasis $\{|n\rangle\}$ as

$$|q'\rangle = \sum_n |n\rangle \langle n|q'\rangle = \sum_n |n\rangle \langle q'|n\rangle^* = \sum_n |n\rangle \phi_n^*(q')$$

where $\phi_n(q')$ is the wavefunction of the energy eigenstate $|n\rangle$ in the position basis. Thus

$$\begin{aligned} G(q'', q', E) &= \langle q''| \frac{1}{E - \hat{H}} \left(\sum_n |n\rangle \phi_n^*(q') \right) \\ &= \sum_n \langle q''| \frac{\phi_n^*(q')}{E - E_n} |n\rangle \\ &= \sum_n \frac{\phi_n(q'')\phi_n^*(q')}{E - E_n} \end{aligned}$$

We now take $q' = q'' \equiv q$ and integrate over all space. This gives

$$\begin{aligned}\int dq\, G(qqE) &= \int dq \sum_n \frac{\phi_n(q)\phi_n^*(q)}{E - E_n} \\ &= \sum_n \frac{1}{E - E_n}\end{aligned} \tag{5}$$

This equation deserves special attention: it says that upon integrating the Green's function with the same initial and final spatial point, the poles of the integral are precisely the energies of the Schrodinger picture energy eigenstates. Together, equations (3) and (5) provide a pathway for extracting the energy levels from the raw propagator. The task is now, naturally, how one could evaluate the somewhat scary-looking propagator (1).

3.3 The Van-Vleck-Gutzwiller approximation

Feynman's path propagator (1), while elegant in principle, raises some practical issues, the most obvious of which being how to actually evaluate an infinite number of integrals. Seldom is the potential nice enough that the exact integrals reduce to workable forms (the most important of these "simple" potentials being of course the harmonic oscillator), but most of the time some sort of approximation method has to be invoked. The Van-Vleck-Gutzwiller approximation is one such method.

Published over the years 1967 to 1971, a series of 4 papers by Martin Gutzwiller developed this approximation method [4, 5, 6, 7]. The result was an *approximation* for the Green's function between a starting point q' and an ending point q''. With this approximated Green's function, we can use (5) to obtain the approximate spectrum of a potential solely from the classically strictly periodic orbits. We will discuss two simple examples, namely the free particle on 1- and 2- torus, in the next section. Gutzwiller originally developed this approximation for atomic physics and did not use it in our context, but these torus examples will help us with the cross well as well. In this section we derive this approximation.

3.3.1 An approximation for the integral in the propagator

We start with the propagator (1). The first task is to work out the integrals

$$\int d^n q_1 \int d^n q_2 ... \int d^n q_{N-1}\, \exp\left(i \frac{R(q_1, q_2, .., q_{N-1})}{\hbar} \right) \tag{6}$$

The Gutzwiller approximation's argument goes as follows: we argued that the only paths that contribute significantly to the overall amplitude are the paths that are sufficiently close

to the true classical path in the classical limit. In light of this, we no longer perform the integration over all paths, but only the paths sufficiently close to the true classical path.

Denote the true classical path as $\{q_0 = q', \bar{q_1}, \bar{q_2}, ..., q_{\bar{N-1}}, q_N = q''\}$, i.e. with a bar. Notice that these barred position quantities are constants. A path that is infinitesimally close to this true classical path is thus given as

$$\{q_0 = q', q_1 = \bar{q_1} + \delta q_1, q_2 = \bar{q_2} + \delta q_2, ..., q_{N-1} = q_{\bar{N-1}} + \delta q_{N-1}, q_N = q''\}$$

at the times t_i.

The action of a path close to the classical true path is therefore a simple Taylor expansion of the true classical action:

$$\begin{aligned} R(q_1, q_2, .., q_{N-1}) &= R(\bar{q_1} + \delta q_1, ..., q_{\bar{N-1}} + \delta q_{N-1}) \\ &= R(\bar{q_1}, .., q_{\bar{N-1}}) + \left[\delta q_1 \frac{\partial R}{\partial q_1} + ... + \delta q_{N-1} \frac{\partial R}{\partial q_{N-1}}\right] \\ &\quad + \frac{1}{2}\left[(\delta q_1)^2 \frac{\partial^2 R}{\partial q_1^2} + ... + (\delta q_{N-1})^2 \frac{\partial^2 R}{\partial q_{N-1}^2} + 2\delta q_1 \delta q_2 \frac{\partial^2 R}{\partial q_1 \partial q_2} + ...\right] + \mathcal{O}(\delta q^3) \\ &\approx \bar{R} + \frac{1}{2}\sum_{jl} R_{jl} \delta q_j \delta q_l \end{aligned}$$

where we drop 3rd order and higher terms since the paths are sufficiently close to the true classical path. In addition, the 1st order term is also zero. This is the definition of the true classical path: the action is stationary with respect to any first order variation for all the partition points. The only surviving terms are the 2nd order terms, and we have defined

$$R_{jl} = \frac{\partial^2 R}{\partial q_j \partial q_l}$$

Note that R_{jl} when viewed as a matrix is real and symmetric, and has size $n(N-1)$-by-$n(N-1)$. And as per our bar convention, $\bar{R}$ is the action of the true classical path (which is a constant with respect to any variation).

The integral (6) is thus

$$\begin{aligned} &\int d^n q_1 \int d^n q_2 ... \int d^n q_{N-1} \exp\left(i \frac{R(q_1, q_2, .., q_{N-1})}{\hbar}\right) \\ &\approx \sum_{\substack{\text{classical} \\ \text{paths}}} \exp\left(\frac{i}{\hbar}\bar{R}\right) \int d^n(\bar{q_1} + \delta q_1) ... \int d^n(q_{\bar{N-1}} + \delta q_{N-1}) \exp\left(\frac{i}{\hbar}\frac{1}{2}\sum_{jl} R_{jl}\delta q_j \delta q_l\right) \\ &= \sum_{\substack{\text{classical} \\ \text{paths}}} \exp\left(\frac{i}{\hbar}\bar{R}\right) \int d^n x_1 ... \int d^n x_{N-1} \exp\left(\frac{i}{\hbar}\frac{1}{2}\sum_{jl} R_{jl} x_j x_l\right) \end{aligned} \tag{7}$$

where in the last step we utilized the fact that $\bar{q}_i$ are constant and thus $d(\bar{q}_i + \delta q_i) = d(\delta q_i)$, and we renamed δq_i to x_i to avoid notation messiness. Because in the integral over all paths, multiple classical paths can arise between two points for the potential in question [4], each carrying its own cluster of close-by paths for Taylor expansion, the integral would reduce to a sum over all of the classical paths.

This integral would be a chain of $n(N-1)$ Gaussian integrals if the matrix R_{jl} were diagonal. We thus make a change of variables to transform the matrix into its principal axes. Let R' be the matrix such that its matrix elements are $R_{jl}/2$. Since R' is real and symmetric, it can be diagonalized as

$$R' = U^T D U$$

where D is a diagonal matrix with the (real) eigenvalues of R' on the diagonal, and $U^T = U^{-1}$. Upon the change of variables

$$x'_m = \sum_j U_{mj} x_j$$

the integral in (7) becomes

$$\begin{aligned} &\sum_{\substack{\text{classical}\\ \text{paths}}} \exp\left(\frac{i}{\hbar}\bar{R}\right) \int d^n x_1 ... \int d^n x_{N-1} \exp\left(\frac{i}{\hbar}\sum_m (x_m)^2 D_{mm}\right) \\ &= \sum_{\substack{\text{classical}\\ \text{paths}}} \exp\left(\frac{i}{\hbar}\bar{R}\right) \left[\int d^n x_1 \exp\left(\frac{i}{\hbar} x_1^2 D_{11}\right)\right] ... \left[\int d^n x_{N-1} \exp\left(\frac{i}{\hbar} x_{N-1}^2 D_{N-1,N-1}\right)\right] \end{aligned} \tag{8}$$

The details of this transform is done in Appendix B. This is now $n(N-1)$ Gaussian integrals. Inspect each Gaussian

$$\int dx \exp\left(\frac{i}{\hbar} x^2 D_{mm}\right)$$

where is integration is performed over all x [5]. In fact, this is *almost* a Gaussian: its exponent is imaginary and we need to be careful about convergence, as D_{mm} (the eigenvalues of R') can be either positive or negative. We make the substitution

$$\begin{cases} u = e^{-i\pi/4} x & \text{if } D_{mm} > 0 \\ u = e^{i\pi/4} x & \text{if } D_{mm} < 0 \end{cases}$$

[4] For example, in a 1D harmonic oscillator, the particle can oscillate from the middle back to the middle in the same amount of time by taking the path on the left half or the right half.

[5] We still perform the Feynman path integral over all possible paths; the fact that only paths close to the classical path participate has already been accounted for by discarding higher order terms in the expansion for the integrand.

For the case of $D_{mm} > 0$, the almost Gaussian integral is now

$$\int e^{i\pi/4} du \, \exp\left(\frac{i}{\hbar} e^{i\pi/2} u^2 D_{mm}\right) = \int e^{i\pi/4} du \, \exp\left(-\frac{D_{mm}}{\hbar} u^2\right) = e^{i\pi/4} \sqrt{\frac{\pi\hbar}{D_{mm}}}$$

which now converges with no problem, since in this case D_{mm} is real and positive. Similarly, for $D_{mm} < 0$, the almost Gaussian integral evaluates to

$$\int e^{-i\pi/4} du \, \exp\left(\frac{i}{\hbar} e^{-i\pi/2} u^2 D_{mm}\right) = \int e^{-i\pi/4} du \, \exp\left(-\frac{|D_{mm}|}{\hbar} u^2\right) = e^{-i\pi/4} \sqrt{\frac{\pi\hbar}{|D_{mm}|}}$$

The integral in (8) is thus a product of $n(N-1)$ such Gaussians. Let M denote the number of negative eigenvalues of the matrix R', i.e. the number of negative D_{mm}s. Inside the square root on the denominator, we have the product of all the eigenvalues of R' (with an absolute value), so it's the absolute value of the determinant of R'. So we have

$$(8) = \sum_{\substack{\text{classical} \\ \text{paths}}} e^{i\left[\frac{\bar{R}}{\hbar} + (n(N-1)-M)\frac{\pi}{4} - M\frac{\pi}{4}\right]} (\sqrt{\pi\hbar})^{n(N-1)} \sqrt{\frac{1}{|\det(R')|}}$$

In terms of the original $R_{jl} = \dfrac{\partial^2 R}{\partial q_j \partial q_l}$, since the elements of R' are $R_{jl}/2$, and R' is a $n(N-1)$-by-$n(N-1)$ matrix, so $\det(R_{jl}) = 2^{n(N-1)} \det(R')$.

The reader who kept track would remember that the integral (8) is an approximation for the one in the propagator (6). Therefore

$$\begin{aligned} &\int d^n q_1 \int d^n q_2 ... \int d^n q_{N-1} \, \exp\left(i \frac{R(q_1, q_2, .., q_{N-1})}{\hbar}\right) \\ &\approx \sum_{\substack{\text{classical} \\ \text{paths}}} (2\pi\hbar)^{\frac{n(N-1)}{2}} |\det(R_{jl})|^{-\frac{1}{2}} e^{i\left[\frac{\bar{R}}{\hbar} + n(N-1)\frac{\pi}{4} - M\frac{\pi}{2}\right]} \end{aligned} \tag{9}$$

M, the number of negative eigenvalues of $R_{jl} = \dfrac{\partial^2 R}{\partial q_j \partial q_l}$, is known as the **Maslov index** of the trajectory.

We now plug this integral back into the propagator (1) and massage a bit the prefactors of

$2\pi\hbar$-s and i-s. The result is

$$K(q''t''q't') \approx \sum_{\substack{\text{classical}\\ \text{paths}}} \lim_{N\to\infty} \left(\frac{m}{2\pi i\hbar\epsilon}\right)^{\frac{nN}{2}} (2\pi\hbar)^{\frac{n(N-1)}{2}} |\det(R_{jl})|^{-\frac{1}{2}} e^{i\left[\frac{\bar{R}}{\hbar}+n(N-1)\frac{\pi}{4}-M\frac{\pi}{2}\right]}$$

$$= \sum_{\substack{\text{classical}\\ \text{paths}}} \lim_{N\to\infty} \left(\frac{m}{\epsilon}\right)^{\frac{nN}{2}} \left(\frac{1}{2\pi i\hbar}\right)^{\frac{n}{2}} |\det(R_{jl})|^{-\frac{1}{2}} e^{i\left(\frac{\bar{R}}{\hbar}-M\frac{\pi}{2}\right)} \tag{10}$$

Notice that we have reduced the evaluation of the propagator from an impractical integral over all paths with all kinds of potential integration measure problems to a doable simple sum over classical paths! The next step is to get rid of the explicit dependence on the discretization N and $\epsilon = \dfrac{t''-t'}{N}$, i.e. we now want to evaluate

$$\lim_{N\to\infty} \left(\frac{m}{\epsilon}\right)^{\frac{nN}{2}} |\det(R_{jl})|^{-\frac{1}{2}} \tag{11}$$

or rather its square

$$\lim_{N\to\infty} \left(\frac{m}{\epsilon}\right)^{nN} |\det(R_{jl})|^{-1} \tag{12}$$

We take this opportunity to clarify a notation convention: when we mean the determinant of a matrix, we will always explicitly use "det". Two vertical bars always indicate absolute value. With this convention, now is a good time to take the mental note that (11) and (12) are always positive.

3.3.2 Evaluating $det(R_{jl})$

We are looking at non relativistic theory. The Lagrangian is the classical one, i.e. kinetic energy minus potential energy, and the action R (no bar!) as a function of the partition points is thus

$$R(q_1, q_2, .., q_{N-1}) = \int_{t'}^{t''} \mathcal{L}\, dt$$

$$= \lim_{N\to\infty} \sum_{i=1}^{N} \epsilon \left[\frac{1}{2} m \left(\frac{q_i - q_{i-1}}{\epsilon}\right)^2 - V(q_i)\right]$$

$$= \lim_{N\to\infty} \sum_{i=1}^{N} \left[\frac{1}{2} m \frac{(q_i - q_{i-1})^2}{\epsilon} - \epsilon V(q_i)\right]$$

where we used ϵ in place of dt in the Riemann sum to conform to our convention. Take mental note of the implicit dependence of ϵ on N. We can now take the derivatives for the matrix elements of R_{jl}. Only two terms in the i sum involve q_l, so

$$\begin{aligned}
\frac{\partial R}{\partial q_l} &= \lim_{N\to\infty} \frac{\partial}{\partial q_l}\left[\frac{1}{2}m\frac{(q_l - q_{l-1})^2}{\epsilon} - \epsilon V(q_l) + \frac{1}{2}m\frac{(q_{l+1} - q_l)^2}{\epsilon} - \epsilon V(q_{l+1})\right] \\
&= \lim_{N\to\infty}\left[\frac{m}{\epsilon}(2q_l - q_{l-1} - q_{l+1}) - \epsilon\frac{\partial V(q_l)}{\partial q_l}\right] \\
\therefore R_{jl} = \frac{\partial^2 R}{\partial q_j \partial q_l} &= \lim_{N\to\infty}\left[\frac{m}{\epsilon}(2\delta_{jl} - \delta_{j,l-1} - \delta_{j,l+1}) - \epsilon\delta_{jl}\frac{\partial^2 V(q_l)}{\partial q_l^2}\right]
\end{aligned}$$

The determinant of this matrix is non-trivially dependent on the potential V, and this is in general the furthest we can go without assuming anything about the potential. We include a simple discussion with an arbitrary potential in one dimension in Appendix C. At this point, Gutzwiller went on to use this approximation method for atomic physics. He wanted to investigate the relationship between classical Kepler orbits in a Coulomb potential and the quantum energy levels [6]. We will be using this approximation in the context of the cross well.

In our cross well, the potential is either zero or infinite. Any classical trajectory would completely be inside the zero potential regions, making our particle a "free" particle, except when bouncing from the walls. We now work out the Gutzwiller approximation in the case of zero potential.

3.3.3 The propagator approximation for the free particle ($V = 0$)

With $V = 0$, the action is

$$\begin{aligned}
R(q_1, q_2, .., q_{N-1}) &= \lim_{N\to\infty}\sum_{i=1}^{N}\left[\frac{1}{2}m\frac{(q_i - q_{i-1})^2}{\epsilon}\right] \\
&= \lim_{N\to\infty}\sum_{n}\sum_{i=1}^{N}\left[\frac{1}{2}m\frac{(q_{i,n} - q_{i-1,n})^2}{\epsilon}\right]
\end{aligned}$$

We have simply decomposed the distance of each partition segment onto the n dimensions. Each dimension is completely independent to the others. We see that upon being hit with two derivatives, R_{jl} has the same form as previously discussed, but with one such triplet of deltas for each dimension:

$$R_{jn,ln} = \frac{\partial^2 R}{\partial q_{jn}\partial q_{ln}} = \lim_{N\to\infty}\left[\frac{m}{\epsilon}(2\delta_{jn,ln} - \delta_{jn,(l-1)n} - \delta_{jn,(l+1)n})\right]$$

The n subscripts are simply denoting that the cross derivatives between different dimensions are always zero. Take for example $n = 3$. Let the rows and columns be displayed in the order q_{1x}, q_{1y}, q_{1z}, q_{2x}, q_{2y}, q_{2z}, ..., $q_{N-1,x}$, $q_{N-1,y}$, $q_{N-1,z}$. The matrix R_{jl} is thus

$$R_{jl} = \lim_{N\to\infty} \frac{m}{\epsilon} \begin{pmatrix} 2 & 0 & 0 & -1 & 0 & 0 & & & & 0 \\ 0 & 2 & 0 & 0 & -1 & 0 & & & & \\ 0 & 0 & 2 & 0 & 0 & -1 & & & & \\ -1 & 0 & 0 & 2 & 0 & 0 & \cdots & & & \\ 0 & -1 & 0 & 0 & 2 & 0 & & & & \\ 0 & 0 & -1 & 0 & 0 & 2 & & & & \\ & & \vdots & & & & \ddots & & & \\ & & & & & & & 2 & 0 & 0 \\ & & & & & & & 0 & 2 & 0 \\ 0 & & & & & & & 0 & 0 & 2 \end{pmatrix}.$$

It is now a straightforward issue of mathematical induction, albeit one needs to quite careful with the N and $N-1$ factors, to show that in n dimensions,

$$\det(R_{jl}) = \left(\frac{m}{\epsilon}\right)^{n(N-1)} N^n$$

We stop writing the $N \to \infty$ limit as it does not really need to be explicit anymore. Notice this determinant is always positive for the zero potential. Expression (12) is thus

$$(12) = \left(\frac{m}{\epsilon}\right)^{nN} |\det(R_{jl})|^{-1} = \frac{m^n}{\epsilon^n N^n} = \left(\frac{m}{t'' - t'}\right)^n$$

and we have eliminated the dependence on the discretization N!

To aid the future approximation to the Green's function, we write this result in a slightly different form. For the free particle, the action can be written down from the endpoints alone without discretization at all, as the kinetic energy is constant:

$$\begin{aligned} R &= \frac{1}{2} m v^2 (t'' - t') \\ &= \frac{1}{2} m (t'' - t') \left[\left(\frac{q_x'' - q_x'}{t'' - t'} \right)^2 + \left(\frac{q_y'' - q_y'}{t'' - t'} \right)^2 ... \right] \\ &= \frac{1}{2} \frac{m}{t'' - t'} \left(\sum_{i=1}^{n} (q_i'' - q_i')^2 \right) \end{aligned}$$

Consider the matrix of the mixed second derivatives of the action with respect to the starting

and ending points

$$\frac{\partial^2 R}{\partial q'' \partial q'} \equiv \begin{pmatrix} \frac{\partial^2 R}{\partial q_x'' \partial q_x'} & \frac{\partial^2 R}{\partial q_x'' \partial q_y'} & \\ \frac{\partial^2 R}{\partial q_y'' \partial q_x'} & \frac{\partial^2 R}{\partial q_y'' \partial q_y'} & \cdots \\ \vdots & & \ddots \end{pmatrix} \tag{13}$$

Any derivative between different dimensions is zero, and all diagonal entries are $-\frac{m}{t''-t'}$. This matrix has dimensions n-by-n. Therefore $\det\left(\frac{\partial^2 R}{\partial q'' \partial q'}\right) = (-1)^n \left(\frac{m}{t''-t'}\right)^n$, and so

$$(12) = (-1)^n \det\left(\frac{\partial^2 R}{\partial q'' \partial q'}\right)$$

Plugging (12) back into (10) gives us the approximated propagator for zero potential regions:

$$K(q''t''q't') \approx \sum_{\substack{\text{classical} \\ \text{paths}}} \left(\frac{1}{2\pi i\hbar}\right)^{\frac{n}{2}} \sqrt{(-1)^n \det\left(\frac{\partial^2 R}{\partial q'' \partial q'}\right)}\, e^{i\left(\frac{\bar{R}}{\hbar} - M\frac{\pi}{2}\right)} \tag{14}$$

In fact, this form of the approximated propagator (14) is not just valid for the free particle. It is also valid for particles in a spherically (or centrally) symmetric potential [4], although we do not have the page space to show it here. For a generic potential, one would have to evaluate $\det(R_{jl})$ from a differential equation obtained via the recursive relation for determinants as discussed in Appendix C.

The final order of business is to find the Maslov index M for the free particle. In fact, for the free particle the Maslov index is easily seen to be zero. M is the number of negative eigenvalues of $R_{jl} = \frac{\partial^2 R}{\partial q_j \partial q_l}$. When viewing the action R as a function of the partition points q_i, we see that R_{jl} is simply the Hessian of R. Since for the free particle the action is always a minimum with respect to variations in the path [6], this Hessian will be positive definite and has all positive eigenvalues.

Therefore, the propagator for the free particle in n dimensions from q' to q'' in time t can be

[6] This can be understood from relativity. The relativistic action of a free particle is $-mc^2$ times the total proper time along its trajectory, and free particle will maximize the proper time.

approximated as

$$K(q''t''q't') \approx \sum_{\substack{\text{classical}\\ \text{paths}}} \left(\frac{1}{2\pi i\hbar}\right)^{\frac{n}{2}} \sqrt{(-1)^n \det\left(\frac{\partial^2 R}{\partial q''\partial q'}\right)}\, e^{i\frac{\bar{R}}{\hbar}} \tag{15}$$

3.3.4 The Green's function approximation for the free particle ($V = 0$)

With the approximated propagator, we can now plug it into the definition of the Green's function (3) and obtain an approximation for the free particle's Green's function.

$$\begin{aligned} G(q'', q', E) &= \frac{1}{i\hbar}\int_0^\infty dt K(q''t, q'0)\exp\left(\frac{iEt}{\hbar}\right) \\ &\approx \sum_{\substack{\text{classical}\\ \text{paths}}} \frac{1}{i\hbar}\left(\frac{1}{2\pi i\hbar}\right)^{\frac{n}{2}} \int_0^\infty dt \sqrt{(-1)^n \det\left(\frac{\partial^2 R}{\partial q''\partial q'}\right)}\, e^{i\frac{\bar{R}+Et}{\hbar}} \end{aligned} \tag{16}$$

This integral can be approximated via the stationary phase integral approximation (see Appendix D). The stationary points t_0 of the phase are

$$\frac{d}{dt}(Et + \bar{R})\bigg|_{t=t_0} = 0, \text{ i.e. } E = -\frac{\partial \bar{R}}{\partial t}\bigg|_{t=t_0}$$

For the free particle covering a distance L, the classical action of the true path is $\bar{R} = mv^2t/2 = mL^2/2t$. The phase function thus has the form $f(t) = Et + b/t$, where E, b and t are all positive. Therefore the phase function has exactly one stationary point t_0, which is a minimum, so the $\text{sign}\{f''(t_0)\} = +1$ in the stationary phase integral approximation. We thus have

$$
\begin{aligned}
G(q'', q', E) &\approx \sum_{\substack{\text{classical}\\ \text{paths}}} \frac{1}{i\hbar}\left(\frac{1}{2\pi i\hbar}\right)^{\frac{n}{2}} \int_0^\infty dt \sqrt{(-1)^n \det\left(\frac{\partial^2 R}{\partial q'' \partial q'}\right)}\, e^{i\frac{\bar{R}+Et}{\hbar}} \\
&= \sum_{\substack{\text{classical}\\ \text{paths}}} \frac{1}{i\hbar}\left(\frac{1}{2\pi i\hbar}\right)^{\frac{n}{2}} \sqrt{(-1)^n \det\left(\frac{\partial^2 R}{\partial q'' \partial q'}\right)}\Bigg|_{t=t_0} e^{\frac{i}{\hbar}[\bar{R}(q'', t_0, q', 0)+Et_0]}\, e^{i\frac{\pi}{4}} \\
&\quad \sqrt{\frac{2\pi\hbar}{\left.\frac{\partial^2[\bar{R}(q'', t, q', 0)+Et]}{\partial t^2}\right|_{t=t_0}}} \\
&= \sum_{\substack{\text{classical}\\ \text{paths}}} \frac{1}{i\hbar(2\pi i\hbar)^{\frac{n-1}{2}}} \sqrt{(-1)^n \det\left(\frac{\partial^2 R}{\partial q'' \partial q'}\right)}\Bigg|_{t=t_0} \left(\left.\frac{\partial^2 \bar{R}}{\partial t^2}\right|_{t=t_0}\right)^{-\frac{1}{2}} e^{\frac{i}{\hbar}[\bar{R}(q'', t_0, q', 0)+Et_0]}
\end{aligned}
$$

What exactly does this t_0 represent? For a classical trajectory from q' to q'', with energy E, initial momentum p' and final momentum p'', the action $\bar{R}$ satisfies the following standard results from classical mechanics

$$
\frac{\partial \bar{R}}{\partial t} = -E, \quad \frac{\partial \bar{R}}{\partial q'} = -p', \quad \frac{\partial \bar{R}}{\partial q''} = p'' \tag{17}
$$

The energy definition is exactly the condition for stationary phase t_0! We see that the phase stationary point t_0 is exactly the time taken for the particle to traverse the classical path. Since in the propagator approximation we are already summing over strictly classical paths, this evaluation over t_0 is actually automatically satisfied. In addition, this also means the phase function $[\bar{R}(q'', t_0, q', 0) + Et_0]$ is simply the Legendre transformed action, or the $\int pdq$ action, which we denote by $S(q'', q', E)$:

$$
S(q'', q', E) = \int_{q'}^{q''} pdq = \bar{R}(q'', t_0, q', 0) + Et_0
$$

Similar relationships to (17) for the R action exist for the S action as well, and can be easily seen from the definition $S = Et + \bar{R}$:

$$
\frac{\partial S}{\partial E} = t, \quad \frac{\partial S}{\partial q'} = -p', \quad \frac{\partial S}{\partial q''} = p'' \tag{18}
$$

Two immediate follow-up results will be useful:

$$
\frac{\partial t}{\partial E} = \frac{\partial^2 S}{\partial E^2}, \quad \frac{\partial^2 \bar{R}}{\partial t^2} = \frac{\partial}{\partial t}(-E) = -\left(\frac{\partial^2 S}{\partial E^2}\right)^{-1} \tag{19}
$$

We are thus left with

$$G(q'', q', E) \approx \sum_{\substack{\text{classical} \\ \text{paths}}} \frac{1}{i\hbar(2\pi i\hbar)^{\frac{n-1}{2}}} \sqrt{(-1)^n \det\left(\frac{\partial^2 R}{\partial q'' \partial q'}\right)} \left(\frac{\partial^2 \bar{R}}{\partial t^2}\right)^{-\frac{1}{2}} e^{\frac{i}{\hbar} S(q'', q', E)} \tag{20}$$

With some maneuvering we can show that

$$\sqrt{(-1)^n \det\left(\frac{\partial^2 R}{\partial q'' \partial q'}\right)} \left(\frac{\partial^2 \bar{R}}{\partial t^2}\right)^{-\frac{1}{2}} = \left| \det \begin{pmatrix} \frac{\partial^2 S}{\partial q'' \partial q'} & \frac{\partial^2 S}{\partial q'' \partial E} \\ \frac{\partial^2 S}{\partial E \partial q'} & \frac{\partial^2 S}{\partial E^2} \end{pmatrix} \right|^{\frac{1}{2}} \tag{21}$$

where on the right hand side the vertical bars denote absolute value, and the matrix is $n+1$ dimensional. The upper left n-by-n corner is the mixed second partial derivatives with respect to the starting and ending point, similar to (13) for R. It might be helpful to write out this matrix explicitly to avoid possible confusion:

$$\begin{pmatrix} \frac{\partial^2 S}{\partial q'' \partial q'} & \frac{\partial^2 S}{\partial q'' \partial E} \\ \frac{\partial^2 S}{\partial E \partial q'} & \frac{\partial^2 S}{\partial E^2} \end{pmatrix} \equiv \begin{pmatrix} \frac{\partial^2 S}{\partial q_x'' \partial q_x'} & \frac{\partial^2 S}{\partial q_x'' \partial q_y'} & \cdots & \frac{\partial^2 S}{\partial q_x'' \partial E} \\ \frac{\partial^2 S}{\partial q_y'' \partial q_x'} & \frac{\partial^2 S}{\partial q_y'' \partial q_y'} & \cdots & \frac{\partial^2 S}{\partial q_y'' \partial E} \\ \vdots & & & \ddots \\ \frac{\partial^2 S}{\partial E \partial q_x'} & \frac{\partial^2 S}{\partial E \partial q_y'} & \cdots & \frac{\partial^2 S}{\partial E^2} \end{pmatrix} \tag{22}$$

(21) can be shown very quickly. With the relations (18) and (19), the right hand side inside the absolute value (discarding the overall square root) is

$$\det \begin{pmatrix} \frac{\partial^2 S}{\partial q'' \partial q'} & \frac{\partial^2 S}{\partial q'' \partial E} \\ \frac{\partial^2 S}{\partial E \partial q'} & \frac{\partial^2 S}{\partial E^2} \end{pmatrix} = \det \begin{pmatrix} -\frac{\partial p'}{\partial q''} & \frac{\partial t}{\partial q''} \\ -\frac{\partial p'}{\partial E} & \frac{\partial t}{\partial E} \end{pmatrix}$$

$$= (-1)^n \frac{\partial(p', t)}{\partial(q'', E)} = (-1)^n \frac{\partial(p', t)}{\partial(q'', t)} \frac{\partial(q'', t)}{\partial(q'', E)} = (-1)^n \underbrace{\det\left(\frac{\partial p'}{\partial q''}\right)}_{\text{n by n}} \underbrace{\det\left(\frac{\partial t}{\partial E}\right)}_{\text{1 by 1}}$$

$$= (-1)^n \det\left(\frac{\partial}{\partial q''}\left(-\frac{\partial \bar{R}}{\partial q'}\right)\right) \frac{\partial^2 S}{\partial E^2} = (-1)^n (-1)^n \det\left(\frac{\partial^2 R}{\partial q'' \partial q'}\right) \left(-\frac{\partial^2 \bar{R}}{\partial t^2}\right)^{-1}$$

which equals the left hand side in absolute value. Also, recall that the left hand side came from (12), which is always positive, and the second derivative of the action with respect to

time is positive as well as discussed earlier. Since the left hand side is always positive, we manually introduce an absolute value on the right hand side, and (21) is proved.

Plugging (21) into (20) gives us the final approximation formula for the Green's function of a free particle [7]:

$$\boxed{G(q'', q', E) \approx \sum_{\substack{\text{classical} \\ \text{paths}}} \frac{1}{i\hbar(2\pi i\hbar)^{\frac{n-1}{2}}} \left| \det \begin{pmatrix} \dfrac{\partial^2 S}{\partial q'' \partial q'} & \dfrac{\partial^2 S}{\partial q'' \partial E} \\ \dfrac{\partial^2 S}{\partial E \partial q'} & \dfrac{\partial^2 S}{\partial E^2} \end{pmatrix} \right|^{\frac{1}{2}} e^{\frac{i}{\hbar} S(q'', q', E)}} \tag{23}$$

Let us summarize what we have done: we have gotten rid of the dependence of all variables other than the starting point q', ending point q'', and the energy E. Given a potential, we can now use (23) to obtain the Green's function between two points, using only the classical paths between the two points and the action $S = \int p\, dq$ along these paths.

The recipe in (5) tells us to take $q' = q'' \equiv q$ in Green's function, integrate over all points q in space, and the poles of the integral will give the energy levels of the potential. We are thus looking at a classical path starting and ending both at the same point q; in other words, we are looking at trajectories that are periodic in coordinate space. Moreover, the trajectories is not only periodic in coordinate space, but also periodic in momentum as well. The integral

$$\int dq\, G(qqE) \approx \int dq \sum_{\substack{\text{classical} \\ \text{paths}}} (...)\, e^{\frac{i}{\hbar} S(q,q,E)}$$

should also be evaluated as a stationary phase approximation. Among all the classical paths starting and ending both at q, the only ones participating in the integral are the ones whose S action is stationary with respect to the integral variable q. However, since q is depended on twice by the phase S, both as the starting point q' and ending point q'', the stationary phase condition is actually a chain rule

$$\frac{\mathrm{d}S(q, q, E)}{\mathrm{d}q} = \frac{\partial S(q'', q', E)}{\partial q'} + \frac{\partial S(q'', q', E)}{\partial q''} = -p' + p'' = 0$$

where we have used (18). The participating paths thus have $p' = p''$, i.e. the initial and final momenta are also the same.

Now that we have developed the Gutzwiller approximation for the free particle, let's apply it to some simple examples to see how it is used.

[7] In fact, this result holds for all centrally symmetric potentials, not just the free particle [4]. We derived it with the free particle for simplicity, as that will be our only use case.

3.4 The free particle on various simple geometries

Consider a free particle. Immediately a problem arises: the integral of the Green's function over all space $\int dq\, G(qqE)$ diverges everywhere since the domain of integration is infinite. While the naive interpretation (that every energy is a valid energy level for the free particle) happens to be correct, we would like to be careful. To resolve this issue, we put the free particle on a torus with standard Euclidean metric, so the total content of space is now finite. The physics does not change: if the torus is big enough, what the particle experiences at the middle of the "lab room" shouldn't change based on what is happening at the walls of the room.

We deal with the 1D and 2D cases separately, as the mathematics in 2D turns out to be somewhat richer.

3.4.1 Free particle on the 1-torus

Consider a 1-torus of spatial content L. The non-relativistic momentum as a function of the energy is simply $p = \sqrt{2mE}$. The S action is

$$S(q'', q', E) = \int_{q'}^{q''} p\, dq = \sqrt{2mE}\, |q'' - q'|$$

where $|q'' - q'|$ is to be interpreted as the total path length, not literally, i.e. if the particle goes through the "wall" of the torus once and comes back to the same coordinate, $|q'' - q'|$ would be L, not zero.

Evaluating the necessary derivatives:

$$\frac{\partial^2 S}{\partial q'' \partial q'} = 0, \quad \frac{\partial^2 S}{\partial q'' \partial E} = \frac{\sqrt{2m}}{2\sqrt{E}}, \quad \frac{\partial^2 S}{\partial E \partial q'} = -\frac{\sqrt{2m}}{2\sqrt{E}}$$

The approximation (23) is (n=1)

$$G(q'', q', E) \approx \sum_{\substack{\text{classical} \\ \text{paths}}} \frac{1}{i\hbar} \sqrt{\frac{m}{2E}}\, e^{\frac{i}{\hbar} S(q'', q', E)}$$

We now take $q' = q''$ and integrate over all space. The classical periodic paths have $|q'' - q'| = |\nu| L$, where ν is an integer, since they are the paths where the particle comes back to the same point through $|\nu|$ "portal"s at the walls of the torus. The absolute value is to denote that the particle can go in either direction. Therefore

$$G(q, q, E) \approx \sum_{\nu=-\infty}^{\infty} \frac{1}{i\hbar} \sqrt{\frac{m}{2E}}\, e^{\frac{i}{\hbar}\sqrt{2mE}|\nu| L} \tag{24}$$

Through various uninteresting algebra, namely geometric series (see Appendix E), we obtain

$$\int_0^L dq\, G(qqE) \approx \sum_{\nu=-\infty}^{\infty} \frac{1}{E - \frac{\hbar^2}{2m}\frac{4\pi^2\nu^2}{L^2}}$$

The poles $E_\nu = \frac{\hbar^2}{2m}\frac{4\pi^2\nu^2}{L^2}, \nu \in \mathbb{Z}$, are thus the Gutzwiller approximation energies.

A couple of remarks on this result:
1. As $L \to \infty$, i.e. as the torus gets bigger, the energy levels become continuous, just like a "true" free particle on a torus the size of the universe.

2. The energies are exactly the energies of a free particle in a box of length L with periodic boundary conditions. From standard quantum mechanics, the free particle wavefunction is $\psi(x) = e^{ikx}$. Periodic boundary condition gives $\psi(x + L) = e^{ik(x+L)} = e^{ikx}$, so $kL = pL/\hbar = 2\nu\pi, \nu \in \mathbb{Z}$. With $E = p^2/2m$, we arrive at the Gutzwiller energies. Our torus is in fact, just such a particle in a box with periodic boundary conditions. This is of course expected: the two walls of the torus of course have the same boundary conditions, as they are literally the same spatial position on a torus.

3. The more pedantic reader might feel uncomfortable that $E = 0$ is an energy level. There is no need for anxiety. When $E = 0$, Schrodinger equation simply says the wavefunction is linear. For the textbook particle in an infinite square well, this is not allowed, as the wavefunction vanishes at the two ends of the well and hence needs to vanish everywhere for it to be linear, and it becomes unnormalizable. Here on the torus there is no such vanishing constraint, and the wavefunction can simply be constant throughout the torus as $\psi(x) = \sqrt{1/L}$.

3.4.2 Free particle in the 1D infinite well

The problem of infinite domain of integration is also lifted if we consider the 1D free particle in an infinite potential well of length L. The S action is the same as that of the torus. The participating classical periodic paths must have the same initial and final momentum, so the path lengths must be $|q'' - q'| = |\nu|2L$, where ν is an integer.

The Green's function approximation is therefore exactly the same as (24) in the 1D torus case, only with $2L$ in the place of L. The Gutzwiller energies are thus $E_\nu = \frac{\hbar^2}{2m}\frac{4\pi^2\nu^2}{(2L)^2} = \frac{\hbar^2}{2m}\frac{\pi^2\nu^2}{L^2}, \nu \in \mathbb{Z}$, as expected.

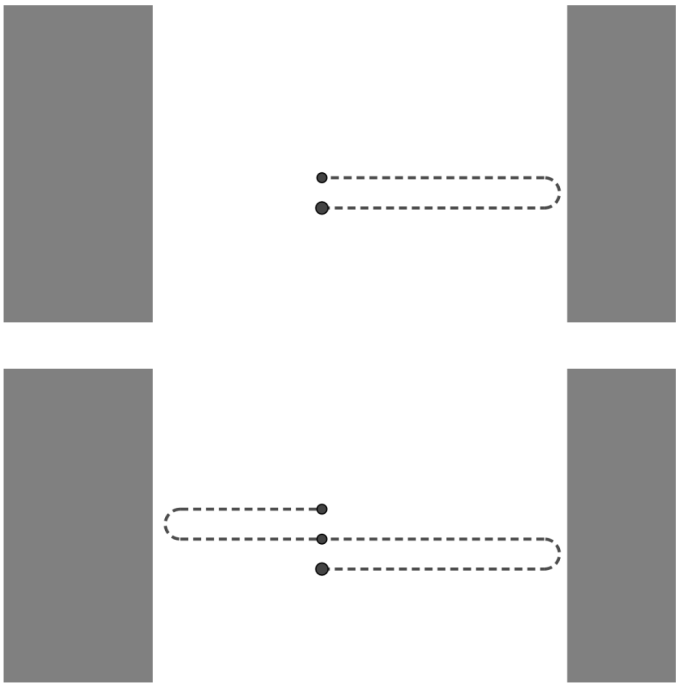

Figure 9: Two types of spatial periodic classical paths in the 1D infinite potential well. Although they both start and end at the same spatial point, only the bottom one is counted in the Green's function approximation's sum. The top path violates the periodic momentum condition, as its initial momentum is to the right, but the final momentum is to the left. Therefore, only classical paths of the bottom type with path length being integer multiples of $2L$, not L, participate in the sum. The potential is a 1D well: the paths and the well are drawn in 2D purely for illustration.

3.4.3 Free particle on the 2-torus

Now we turn to a free particle on a 2-torus with spatial content L^2, i.e. side lengths L. The S action is again given by

$$S(q'', q', E) = \int_{q'}^{q''} p\, dq = \sqrt{2mE}\, |q'' - q'|$$

The periodic classical paths now satisfy

$$\begin{cases} q''_x = q'_x + n_x L \\ q''_y = q'_y + n_y L \end{cases}$$

where there is no restriction on the n_x and n_y other than that they are integers. The rational ratio n_x/n_y encodes the direction of the particle's travel. There is no fear of different starting

and ending momenta when bouncing from any sort of walls like in the 1D infinite well, since there are no walls, and the momentum stays constant as long as n_x/n_y is fixed.

The path length of each periodic classical path is thus given by

$$|q'' - q'| = \sqrt{(q''_x - q'_x)^2 + (q''_y - q'_y)^2} = \sqrt{n_x^2 + n_y^2}L$$

This gives us the S action. Summing over all periodic classical paths, the Green's function approximation in (23) ($n = 2$), keeping in mind the definition of the cross derivative determinant (22), is thus

$$G(q, q, E) \approx -\frac{e^{i\frac{\pi}{4}}}{\sqrt{2\pi}}\frac{m}{\hbar^2}\sum_{n_x,n_y}\sqrt{\frac{\hbar}{L\sqrt{2mE}\sqrt{n_x^2+n_y^2}}}\,e^{\frac{i}{\hbar}L\sqrt{2mE}\sqrt{n_x^2+n_y^2}}$$

(The more diligent reader who is actually working through these equations alongside the author instead of just passively nodding along would notice the importance of the manually inserted absolute value in (23) here.)

Upon integrating over all space on the 2-torus, we have an extra factor of L^2:

$$\int_0^L d^2q\, G(qqE) \approx -\frac{e^{i\frac{\pi}{4}}}{\sqrt{2\pi}}\frac{mL^2}{\hbar^2}\sum_{n_x,n_y}\sqrt{\frac{\hbar}{L\sqrt{2mE}\sqrt{n_x^2+n_y^2}}}\,e^{\frac{i}{\hbar}L\sqrt{2mE}\sqrt{n_x^2+n_y^2}} \tag{25}$$

Unlike the 1D torus, this time the integral (25) is very hard, if not impossible, to rewrite into the exact pole form given by (5). We approximate the poles of (25) by the following rationale: this expression is the sum of many complex numbers labeled by n_x and n_y. The sum will diverge only when the complex numbers line up in phase; otherwise the phases will destructively interfere and the sum will be some finite value, since the magnitude decreases as n_x and n_y increase. When the complex numbers do constructively interfere and the phases line up, the magnitude of the series goes as $n_x^{-1/2}$, so the sum will diverge.

The condition that the phases line up means that when n_x or n_y increase by 1, i.e. when we look at the next term of the series, the phase $\frac{L\sqrt{2mE}}{\hbar}\sqrt{n_x^2+n_y^2}$ need to change by an integer multiple of 2π. We approximate this by taking the derivative of the phase with respect to n_x and n_y, since

$$\frac{d(\text{phase})}{dn_x}dn_x = d(\text{phase})$$

and for large values of n_x, which is the majority of the series, the approximation $dn_x \approx 1$ is

more or less not problematic. The condition for (25) to diverge is thus

$$\begin{cases} \dfrac{\partial}{\partial n_x}\dfrac{L\sqrt{2mE}}{\hbar}\sqrt{n_x^2+n_y^2} = 2\pi\nu_x \\ \dfrac{\partial}{\partial n_y}\dfrac{L\sqrt{2mE}}{\hbar}\sqrt{n_x^2+n_y^2} = 2\pi\nu_y \end{cases}$$

where ν_x and ν_y are (independent) integers. Therefore

$$\frac{L\sqrt{2mE}}{\hbar}\frac{n_x}{\sqrt{n_x^2+n_y^2}} = 2\pi\nu_x, \quad \frac{L\sqrt{2mE}}{\hbar}\frac{n_y}{\sqrt{n_x^2+n_y^2}} = 2\pi\nu_y \tag{26}$$

Squaring these two equations and adding them gives

$$\frac{2mL^2E}{\hbar^2} = 4\pi^2(\nu_x^2+\nu_y^2)$$

so the Gutzwiller energies for a free particle on a 2-torus is thus

$$E = \frac{\hbar^2}{2m}\frac{4\pi^2}{L^2}(\nu_x^2+\nu_y^2)$$

which is the correct result. Like the free particle on the 1-torus, the "extra" factor of 4 in the numerator from the particle in a 2D infinite well comes from the periodic boundary conditions if one were to solve the Schrodinger equation directly. Also like the 1-torus, the spectrum becomes continuous if the torus size L goes to infinity.

If the two sides of the 2-torus have different lengths, with a length of a in the x direction and a length of b in the y direction, i.e. if the classical periodic paths are

$$\begin{cases} q_x'' = q_x' + n_x a \\ q_y'' = q_y' + n_y b \end{cases}$$

Then

$$\int_0^a\int_0^b d^2q\, G(qqE) \approx -\frac{e^{i\frac{\pi}{4}}}{\sqrt{2\pi}}\frac{mab}{\hbar^2}\sum_{n_x,n_y}\sqrt{\frac{\hbar}{\sqrt{2mE}\sqrt{n_x^2a^2+n_y^2b^2}}}\,e^{\frac{i}{\hbar}\sqrt{2mE}\sqrt{n_x^2a^2+n_y^2b^2}}$$

A similar analysis to line up the phases gives the Gutzwiller energies as

$$E = \frac{\hbar^2}{2m}\frac{4\pi^2}{ab}\left(\frac{b}{a}\nu_x^2+\frac{a}{b}\nu_y^2\right) \tag{27}$$

where ν_x and ν_y are independent integers. Again, this agrees with the expected result from directly solving the Schrodinger equation.

3.4.4 Free particle in a 2D infinite channel

We are finally in a position to investigate Schult's claim that quantum bound states arise as a result of classically bounded paths, upon which a shadow of doubt was cast by the potential in figure 3. This potential is an infinite well of width b in the y direction, and a free particle in the x direction. As per our usual method, we imagine the x direction as a torus, and denote the size of the torus by a. As discussed in section 2, if a wavefunction has energy larger than (or equal to) the threshold

$$E_t = \frac{\hbar^2\pi^2}{2mb^2}$$

then it will be an unbound state and scatter throughout the entire channel.

The classical periodic paths are

$$\begin{cases} q_x'' = q_x' + n_x a \\ q_y'' = q_y' + n_y 2b \end{cases}$$

Similar to the particle in the 1D infinite well, because the starting and ending position and momentum of the classical paths that participate in $G(qqE)$ need to be the same, the path length in the y direction must be a integer multiple of $2b$. See figure 10.

The energies of this potential are thus (27) but with $2b$ in place of b:

$$E = \frac{\hbar^2}{2m}\frac{4\pi^2}{a(2b)}\left(\frac{2b}{a}\nu_x^2 + \frac{a}{2b}\nu_y^2\right) = \frac{\hbar^2}{2m}\frac{4\pi^2}{a^2}\nu_x^2 + \frac{\hbar^2}{2m}\frac{\pi^2}{b^2}\nu_y^2 \tag{28}$$

The potential on the torus approaches the true infinite channel when we take $a \to \infty$, in which case the energies become

$$E = \lim_{a\to\infty} \frac{\hbar^2}{2m}\frac{4\pi^2}{a^2}\nu_x^2 + \frac{\hbar^2}{2m}\frac{\pi^2}{b^2}\nu_y^2$$

The first term, which is non-negative, gives a continuum of scattering states in the x direction, none of which has an energy smaller than the threshold $E_t = \hbar^2\pi^2/2mb^2$! Therefore, this infinite channel potential does not have any bound states, and all states are scattering.

The suspicious classical bounded paths that just bounce vertically back and forth on the same x (colored red on figure 3) simply have $q_x'' = q_x'$ and hence $n_x = 0$, which simply gives $\nu_x = 0$ by (26). This is alright, as if a state has an energy the same as the threshold, it is still unbound. In fact this is what is supposed to happen: the state that has exactly the threshold energy is very state that is the ground state of the infinite well in the y direction, and constant in the x direction.

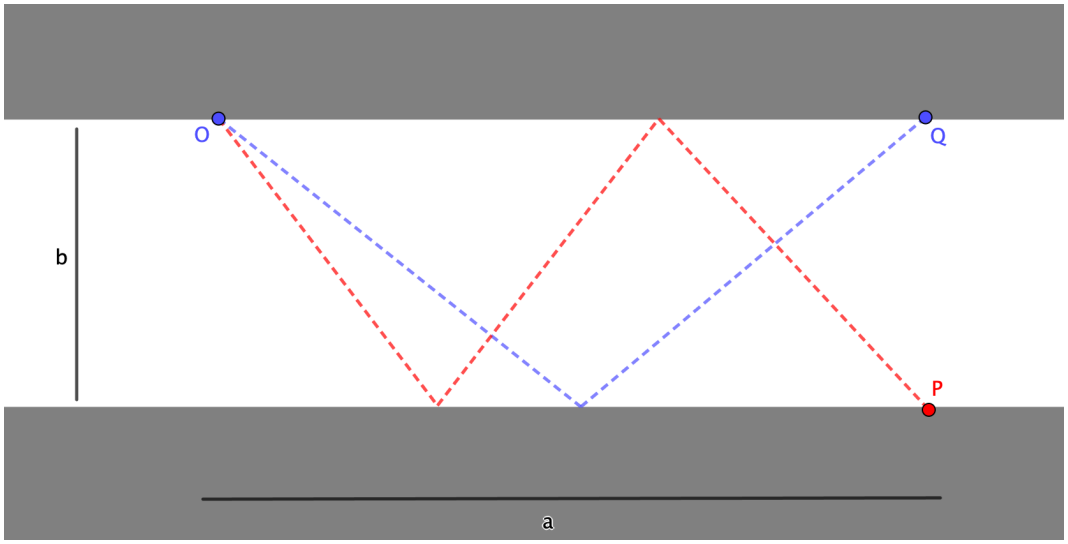

Figure 10: An infinite channel in 2 dimensions, with the x dimension being a torus of length a and the y dimension being an infinite potential well of width b. Because the y dimension has hard walls instead of another torus wall, only point Q is identified as the same point as O, and point P is not. Therefore, the classical paths that start and end both at point O are only the ones that are similar to the blue one, who traverse b vertically an even number of times. The red paths that traverse b an odd number of times are not classically periodic paths.

3.5 The cross well

At last, we are ready to apply the Gutzwiller approximation to our original cross well. We imagine 2-space to be a torus.

When integrating over all space in $\int dq\, G(qqE)$, whose poles we are trying to find, there are two kinds of different points q: the ones in the arms, and the ones in the central square. For any point in the arms, the periodic classical paths starting and ending at that point are identical to those for a point in an infinite 2D channel in the previous section, and they produce a continuum of scattering states and give rise to no bound states. While it is true that a classical path can start in the horizontal arm, bounce into the vertical arm, and then bounce back into the horizontal arm back to its starting point, the fact remains that any such paths that cross the walls of the torus will have energies depending on the torus size L as L^{-2}, and these states will be in a scattering continuum when the torus is large enough.

We thus only need to look at points in the central square. The introduction of an intersection at an otherwise smooth infinite channel creates two diagonal classical periodic trajectories a particle can take. A particle can now bounce off the opposite corners of the intersection and

stay in the central square infinitely without ever flying off to the edges of the torus.

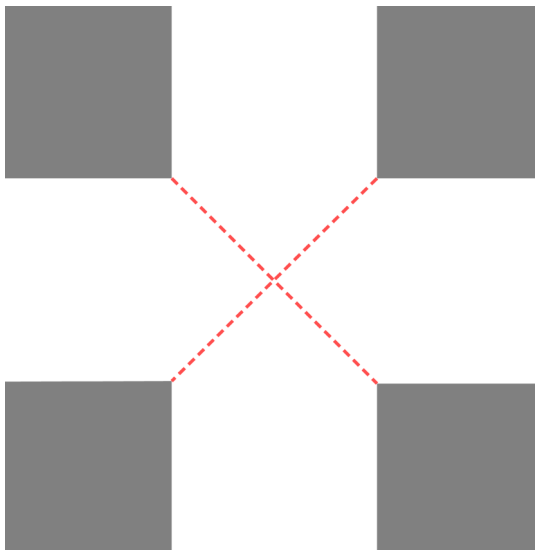

Figure 11: The periodic classical paths in the central square of the cross well. The paths just bounce between opposite corners and do not fly off to the edge of the torus.

As the points with these two newly introduced classical periodic paths only constitute lines and cannot be reasonably integrated over $\int d^2q$, we extend the corners into tiny platforms with length $\sqrt{2}\epsilon$. Denote the width of each channel as a. The geometry is shown as follows:

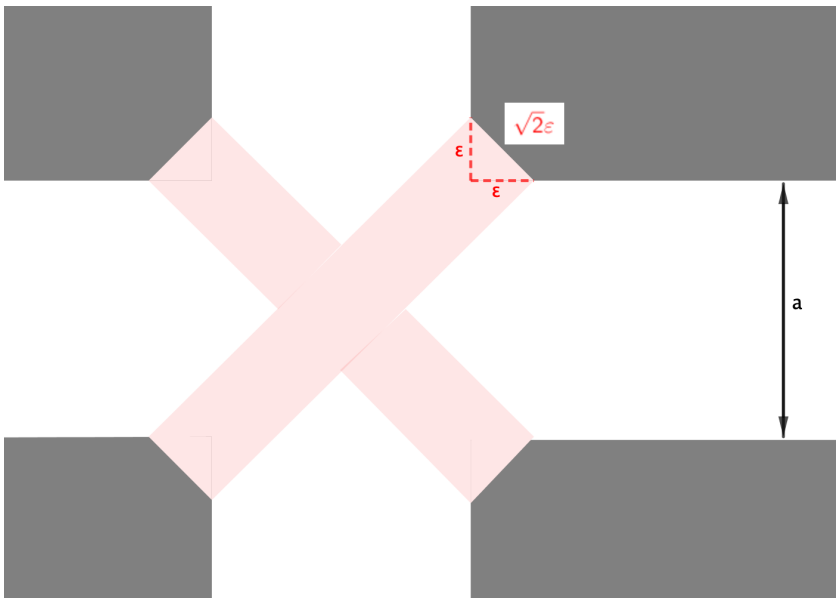

Figure 12: By flattening out the corners, we now have a 2D region of points, instead of two 1D line of points, that has periodic classical paths that bounce between the corners.

We can now integrate over these two diagonal rectangles. The path length for one period along a diagonal path is $|q'' - q'| = 2\sqrt{2}(a+\epsilon)$. We thus have

$$\int d^2q\, G(qqE) \approx -\frac{e^{i\frac{\pi}{4}}}{\sqrt{2\pi}}\frac{m}{\hbar^2}(4a\epsilon + 2\epsilon^2)\sum_\nu \sqrt{\frac{\hbar}{\sqrt{2mE}\nu 2\sqrt{2}(a+\epsilon)}}\, e^{\frac{i}{\hbar}\sqrt{2mE}\nu 2\sqrt{2}(a+\epsilon)} + \text{terms coming from the points in the arms}$$

The integral diverges when the phases line up and constructively interfere, i.e.

$$\frac{\partial}{\partial \nu}\frac{\sqrt{2mE}}{\hbar}\nu 2\sqrt{2}(a+\epsilon) = 2\pi n$$

where n is an integer. This gives the Gutzwiller energies of the cross well as

$$E = \lim_{\epsilon\to 0}\frac{\hbar^2}{2m}\frac{\pi^2 n^2}{2(a+\epsilon)^2} = \frac{\hbar^2}{2m}\frac{\pi^2 n^2}{2a^2} \tag{29}$$

The first three states are given by

$$E_0 = \frac{\hbar^2}{2m}\frac{\pi^2}{2a^2},\quad E_1 = \frac{\hbar^2}{2m}\frac{4\pi^2}{2a^2},\quad E_2 = \frac{\hbar^2}{2m}\frac{9\pi^2}{2a^2}$$

Comparing with the threshold of $E_{\text{t, even}} = \dfrac{\hbar^2}{2m}\dfrac{\pi^2}{a^2}$ for even states and $E_{\text{t, odd}} = \dfrac{\hbar^2}{2m}\dfrac{4\pi^2}{a^2}$ for odd states (see section 2), we see that

$$E_0 < E_{\text{t, even}} < E_1 < E_{\text{t, odd}} < E_2 < E_3 < ...$$

and we have recovered the two bound states, with one even and one odd, of the original cross well!

The Gutzwiller approximated ground and first excited energies are reported as $E_0 = 0.5E_{\text{t, even}}$ and $E_1 = 2E_{\text{t, even}}$. The exact results computed numerically reported by Schult was $E_0 = 0.66E_{\text{t, even}}$ and $E_1 = 3.72E_{\text{t, even}}$ [1]. Quantitatively the Gutzwiller energies are not overly accurate, but as a rough approximation, qualitatively the Gutzwiller approximation provides a rationale as to why the open-ended cross well could host bound states in principle, and allows us to retrieve some information about the potential without feeding it into a computer. In similar open-ended potentials with classical bounded periodic paths, we can now somewhat confidently predict the existence of quantum bound states with this method.

The bound states arise because of the factor of 2 in the denominator of (29), which ultimately come from the $\sqrt{2}\epsilon$ when we flattened the corners. Had we chosen a slightly different geometry to flatten the corners, we would have gotten slightly different numerical energies that could perhaps better match the energies reported by Schult. We leave this work as potential future investigations to those who are interested.

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Appendix A

We wish to evaluate the integral

$$\int_0^\infty r dr \int_0^{2\pi} d\phi \left(N \cos\left(\frac{\pi}{2r_0} r\right) u(-r+r_0) \right) \left[-\frac{\hbar^2}{2\mu} N \left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} \right) \cos\left(\frac{\pi}{2r_0} r\right) u(-r+r_0) \right]$$

Expanding the derivatives with product rule, noting that

$$\frac{\partial}{\partial r} u(-r+r_0) = -\delta(-r+r_0)$$

this integral becomes

$$\begin{aligned}
-\frac{\hbar^2}{2\mu} N^2 2\pi \int_0^{r_0} dr \Bigg[& \\
& - \frac{\pi^2}{4{r_0}^2} r \cos^2\left(\frac{\pi}{2r_0} r\right) u(-r+r_0) && \text{(A.1)} \\
& + \frac{\pi}{r_0} r \cos\left(\frac{\pi}{2r_0} r\right) \sin\left(\frac{\pi}{2r_0} r\right) \delta(-r+r_0) && \text{(A.2)} \\
& - r \cos^2\left(\frac{\pi}{2r_0} r\right) \frac{\mathrm{d}}{\mathrm{d}r} \delta(-r+r_0) && \text{(A.3)} \\
& - \frac{\pi}{2r_0} \cos\left(\frac{\pi}{2r_0} r\right) \sin\left(\frac{\pi}{2r_0} r\right) u(-r+r_0) && \text{(A.4)} \\
& - \cos^2\left(\frac{\pi}{2r_0} r\right) \delta(-r+r_0) \Bigg] && \text{(A.5)}
\end{aligned}$$

Terms (A.2) and (A.5) immediately equal zero because they have

$$\cos\left(\frac{\pi}{2r_0} r\right) \delta(-r+r_0)$$

which is zero for $r \neq r_0$ due to the Delta and also zero for $r = r_0$ due to the $\cos(\pi/2)$.

Term (A.3) is also zero. The derivative of the Delta is treated with integration by parts:

$$\begin{aligned}
& \int_0^{r_0} dr\, r \cos^2\left(\frac{\pi}{2r_0} r\right) \frac{\mathrm{d}}{\mathrm{d}r} \delta(-r+r_0) \\
&= r \cos^2\left(\frac{\pi}{2r_0} r\right) \delta(-r+r_0) - \int_{r=0}^{r_0} dr\, \delta(-r+r_0) \frac{\mathrm{d}}{\mathrm{d}r} \left(r \cos^2 \frac{\pi r}{2r_0} \right) \\
&= 0
\end{aligned}$$

The boundary term is zero again because it contains $\cos(\pi r/2r_0)\delta(-r+r_0)$. The second integral is zero because the derivative by product rule splits into $\cos^2(\pi r/2r_0)$ and $2r\cos(\pi r/2r_0)$ (times some chain rule factors), both of which gives zero when multiplied by the $\delta(-r+r_0)$ outside.

The remaining terms (A.1) and (A.4) both contain $u(-r+r_0)$, which is just one on the integration interval $[0, r_0]$. The integral we seek thus reduces to

$$-\frac{\hbar^2}{2\mu}N^2 2\pi \int_0^{r_0} dr \left[-\frac{\pi^2}{4{r_0}^2}\, r\cos^2\left(\frac{\pi}{2r_0}r\right) - \frac{\pi}{2r_0}\cos\left(\frac{\pi}{2r_0}r\right)\sin\left(\frac{\pi}{2r_0}r\right) \right]$$

which is now trivial. Performing this integral gives the result stated in the main text.

Appendix B

The diagonalization is given as $R' = U^T D U$, where the components of R' are $R_{jl}/2$. In component form, this diagonalization is

$$\begin{aligned}\frac{1}{2}R_{jl} &= \sum_{mn}(U^T)_{jm}D_{mn}U_{nl} \\ &= \sum_{mn}U_{mj}D_{mn}U_{nl} \\ &= \sum_{m}U_{mj}D_{mm}U_{ml}\end{aligned}$$

since D_{mn} is diagonal, i.e. the only surviving term of the n sum is the term with $n = m$. Thus

$$\begin{aligned}\left(\frac{1}{2}R_{jl}\right)x_j x_l &= \sum_{m}U_{mj}D_{mm}U_{ml}x_j x_l \\ &= \sum_{m}(U_{mj}x_j)D_{mm}(U_{ml}x_l)\end{aligned}$$

With the transformation

$$x'_m = \sum_j U_{mj}x_j$$

the exponent of the integrand of (7) is

$$\begin{aligned}\frac{i}{\hbar}\frac{1}{2}\sum_{jl}R_{jl}x_j x_l &= \frac{i}{\hbar}\sum_{jl}\sum_{m}(U_{mj}x_j)D_{mm}(U_{ml}x_l) \\ &= \frac{i}{\hbar}\sum_{m}x'_m D_{mm}x'_m \\ &= \frac{i}{\hbar}\sum_{m}(x'_m)^2 D_{mm}\end{aligned}$$

So the integral (7) is (up to the summation over classical path)

$$\begin{aligned}&\exp\left(\frac{i}{\hbar}\bar{R}\right)\int d^n x_1 ... \int d^n x_{N-1}\,\exp\left(\frac{i}{\hbar}\frac{1}{2}\sum_{jl}R_{jl}x_j x_l\right) \\ &= \exp\left(\frac{i}{\hbar}\bar{R}\right)\int d^n x_1 ... \int d^n x_{N-1}\exp\left(\frac{i}{\hbar}\sum_{m}(x'_m)^2 D_{mm}\right) \\ &= \exp\left(\frac{i}{\hbar}\bar{R}\right)\int d^n x'_1 ... \int d^n x'_{N-1}\exp\left(\frac{i}{\hbar}\sum_{m}(x'_m)^2 D_{mm}\right)\left|\frac{\partial(x_1,...,x_{N-1})}{\partial(x'_1,...,x'_{N-1})}\right|\end{aligned}$$

We now take $n = 1$ for illustrative convenience, though in higher spatial dimensions the argument is exactly the same (with $n(N-1)$ integrals instead of $(N-1)$ integrals). The Jacobian is

$$\left|\frac{\partial(x_1,...,x_{N-1})}{\partial(x'_1,...,x'_{N-1})}\right| = \begin{vmatrix} \frac{\partial x_1}{\partial x'_1} & \frac{\partial x_1}{\partial x'_2} & \cdots & \frac{\partial x_1}{\partial x'_{N-1}} \\ \frac{\partial x_2}{\partial x'_1} & \frac{\partial x_2}{\partial x'_2} & \cdots & \frac{\partial x_2}{\partial x'_{N-1}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial x_{N-1}}{\partial x'_1} & \frac{\partial x_{N-1}}{\partial x'_2} & \cdots & \frac{\partial x_{N-1}}{\partial x'_{N-1}} \end{vmatrix}$$

The transformation $x'_m = \sum_j U_{mj} x_j$ can be written in matrix form as $\mathbf{x}' = U\mathbf{x}$. Because $U^T = U^{-1}$, we have $\mathbf{x} = U^{-1}\mathbf{x}' = U^T\mathbf{x}'$, i.e. $x_m = \sum_j U_{jm} x'_j$, therefore $\frac{\partial x_m}{\partial x'_j} = U_{jm}$. The Jacobian is thus

$$\left|\frac{\partial(x_1,...,x_{N-1})}{\partial(x'_1,...,x'_{N-1})}\right| = \begin{vmatrix} U_{11} & U_{21} & \cdots & U_{N-1,1} \\ U_{12} & U_{22} & \cdots & U_{N-1,2} \\ \vdots & \vdots & \ddots & \vdots \\ U_{1,N-1} & U_{2,N-1} & \cdots & U_{N-1,N-1} \end{vmatrix} = \left|U^T\right| = |U|$$

Since $U^T = U^{-1}$, we have $|U| = \left|U^T\right| = |U^{-1}| = (|U|)^{-1}$, so $|U| = 1$. This is also immediately obvious from the diagonalization, as U is a (real) change of basis matrix and is thus orthogonal. The Jacobian is thus one, so the integral (7) is

$$\exp\left(\frac{i}{\hbar}\bar{R}\right) \int d^n x'_1 ... \int d^n x'_{N-1} \exp\left(\frac{i}{\hbar}\sum_m (x'_m)^2 D_{mm}\right)$$

Renaming the integration variables by removing the primes gives the integral as stated in (8).

Appendix C

$$R_{jl} = \lim_{N\to\infty}\left[\frac{m}{\epsilon}(2\delta_{jl} - \delta_{j,l-1} - \delta_{j,l+1}) - \epsilon\delta_{jl}\frac{\partial^2 V(q_l)}{\partial q_l^2}\right]$$

The matrix whose determinant we want is thus tridiagonal:

$$R_{jl} = \lim_{N\to\infty}$$
$$\begin{pmatrix}
\frac{2m}{\epsilon} - \epsilon\frac{\partial^2 V(q_1)}{\partial q_1^2} & -\frac{m}{\epsilon} & & & & 0 \\
-\frac{m}{\epsilon} & \frac{2m}{\epsilon} - \epsilon\frac{\partial^2 V(q_2)}{\partial q_2^2} & -\frac{m}{\epsilon} & & & \\
 & \ddots & & & & \\
 & & \ddots & & & \\
 & & -\frac{m}{\epsilon} & \frac{2m}{\epsilon} - \epsilon\frac{\partial^2 V(q_{N-2})}{\partial q_{N-2}^2} & -\frac{m}{\epsilon} & \\
0 & & & -\frac{m}{\epsilon} & \frac{2m}{\epsilon} - \epsilon\frac{\partial^2 V(q_{N-1})}{\partial q_{N-1}^2} &
\end{pmatrix}$$

We are discussing a simple one-dimensional example ($n = 1$). We thus have

$$\det(R_{jl}) = \left(\frac{m}{\epsilon}\right)^{(N-1)} \det(R'')$$

where, with $p_i \equiv \frac{\partial^2 V(q_i)}{\partial q_i^2}$,

$$R'' = \frac{\epsilon}{m}R_{jl}$$

$$= \lim_{N\to\infty}\begin{pmatrix}
2 - \frac{\epsilon^2}{m}p_1 & -1 & & & & 0 \\
-1 & 2 - \frac{\epsilon^2}{m}p_2 & -1 & & & \\
 & \ddots & & & & \\
 & & \ddots & & & \\
 & & -1 & 2 - \frac{\epsilon^2}{m}p_{N-2} & -1 & \\
0 & & & -1 & 2 - \frac{\epsilon^2}{m}p_{N-1} &
\end{pmatrix}$$

The determinant of R'' can be evaluated as follows. Let D_k denote the determinant of the lower-right corner of R'' with the top left item being $2 - \epsilon^2 p_k/m$. The determinant of R'' is now just D_1. Evaluating the determinant D_k along its top row gives us the recursive relation

$$D_k = (2 - \frac{\epsilon^2}{m} p_k) D_{k+1} - D_{k+2} \tag{C.1}$$

For example, take the case with $k = 1$. Denote the diagonal elements simply by a_i. We have

$$\begin{aligned}
D_1 &= \det \begin{pmatrix} a_1 & -1 & & & \\ -1 & a_2 & -1 & & \\ & -1 & a_3 & -1 & \\ & & -1 & a_4 & -1 \\ & & & & \ddots \end{pmatrix} \\
&= a_1 \det \begin{pmatrix} a_2 & -1 & & & \\ -1 & a_3 & -1 & & \\ & -1 & a_4 & -1 & \\ & & & \ddots & \end{pmatrix} - (-1) \det \begin{pmatrix} -1 & -1 & & & \\ 0 & a_3 & -1 & & \\ & -1 & a_4 & -1 & \\ & & & \ddots & \end{pmatrix} \\
&= a_1 D_2 + \left[(-1) \det \begin{pmatrix} a_3 & -1 & \\ -1 & a_4 & -1 \\ & & \ddots \end{pmatrix} - (-1) \det \begin{pmatrix} 0 & \dots & \\ 0 & \dots & \\ & & \ddots \end{pmatrix} \right] \\
&= a_1 D_2 - D_3
\end{aligned}$$

The full formula follows naturally from mathematical induction.

With the recursive relation (C.1), we can view the D_k-s as a sequence of numbers indexed with k. In particular, we can view them as samples of a continuous function $D(\tau)$. The samples are defined by $D_k = D((k-1)\epsilon)$, i.e. with sampling period ϵ. This is to make $D(0) = D_1 = \det(R'')$. Similarly, the sequence of numbers p_k can also be viewed as samples of a continuous function $p(\tau)$. The recursive relation (C.1) is now

$$D((k-1)\epsilon) = \left[2 - \frac{\epsilon^2}{m} p((k-1)\epsilon) \right] D(k\epsilon) - D((k+1)\epsilon)$$

$$\therefore \frac{D((k-1)\epsilon) - 2D(k\epsilon) + D((k+1)\epsilon)}{\epsilon^2} = -\frac{1}{m} p((k-1)\epsilon) D(k\epsilon)$$

which, in the limit of $N \to \infty$, i.e. $\epsilon = \dfrac{t'' - t'}{N} \to 0$, turns into a differential equation

$$\frac{\mathrm{d}^2 D(\tau)}{\mathrm{d}\tau^2} + \frac{1}{m} p(\tau) D(\tau) = 0 \tag{C.2}$$

Solving for $D(\tau = 0)$ in (C.2) thus gives the desired $\det(R'')$.

This is as far as we can go for an arbitrary potential. We now have the recipe for the Gutzwiller approximation (in one dimension):

1. From the potential, calculate $p_i \equiv \dfrac{\partial^2 V(q_i)}{\partial q_i^2}$ and its continuous function sibling $p(\tau)$, either through reconstruction samplings from standard signal analysis techniques or other means. Slight inaccuracies in this step is tolerable: this is after all an approximation method.
2. Solve for $D(0) = \det(R'')$ in (C.2), and calculate $\det(R_{jl}) = \left(\dfrac{m}{\epsilon}\right)^{(N-1)} \det(R'')$.
3. Calculate the approximated propagator with (10), where only classical trajectories are involved.
4. Extract the approximated energy levels with the Green's function via (3) and (5).

In higher dimensions, the tridiagonal matrix elements would themselves be n-by-n diagonal matrices, making the differential equation more complicated.

The reader is invited to try out this method on the harmonic oscillator.

Appendix D

The stationary phase approximation is a mathematical tool to approximate integrals of the form

$$I = \int_a^b g(t) e^{ikf(t)} dt$$

Suppose the phase function $f(t)$ has n stationary points with respect to the integration variable t between a and b denoted by s_j, $j = 1, 2, .., n$, i.e.

$$\left.\frac{\mathrm{d}f(t)}{\mathrm{d}t}\right|_{t=s_j} = 0$$

Then

$$I \approx \sum_{j=1}^{n} g(s_j) \exp\left(ikf(s_j) + \mathrm{sign}\{f''(s_j)\}\, i\frac{\pi}{4}\right) \sqrt{\frac{2\pi}{k|f''(s_j)|}}$$

where

$$\mathrm{sign}\{x\} = \begin{cases} +1 & \text{if } x \text{ positive} \\ -1 & \text{if } x \text{ negative} \\ 0 & \text{if } x = 0 \end{cases}$$

i.e. literally the sign of the argument.

This approximation gets better as $k \to \infty$. In the Green's function approximation (16), the role of k is taken by $\frac{1}{\hbar}$, which is very big, so this approximation is valid.

Appendix E

The sum is done via geometric series.

$$
\begin{aligned}
G(q,q,E) &\approx \sum_{\nu=-\infty}^{\infty} \frac{1}{i\hbar}\sqrt{\frac{m}{2E}}\, e^{\frac{i}{\hbar}\sqrt{2mE}|\nu|L} \\
&= \frac{1}{i\hbar}\sqrt{\frac{m}{2E}}\,(1+2\sum_{\nu=1}^{\infty} e^{\frac{i}{\hbar}\sqrt{2mE}\nu L}) \\
&= \frac{1}{i\hbar}\sqrt{\frac{m}{2E}}\,(1+\frac{2e^{\frac{i}{\hbar}\sqrt{2mE}L}}{1-e^{\frac{i}{\hbar}\sqrt{2mE}L}}) \\
&= \frac{1}{i\hbar}\sqrt{\frac{m}{2E}}\,\frac{1+e^{\frac{i}{\hbar}\sqrt{2mE}L}}{1-e^{\frac{i}{\hbar}\sqrt{2mE}L}} \\
&= \frac{1}{i\hbar}\sqrt{\frac{m}{2E}}\,\frac{e^{\frac{i}{2\hbar}\sqrt{2mE}L}(e^{-\frac{i}{2\hbar}\sqrt{2mE}L}+e^{\frac{i}{2\hbar}\sqrt{2mE}L})}{e^{\frac{i}{2\hbar}\sqrt{2mE}L}(e^{-\frac{i}{2\hbar}\sqrt{2mE}L}-e^{\frac{i}{2\hbar}\sqrt{2mE}L})} \\
&= \frac{1}{i\hbar}\sqrt{\frac{m}{2E}}\,\frac{2\cos\left(\frac{\sqrt{2mE}L}{2\hbar}\right)}{-2i\sin\left(\frac{\sqrt{2mE}L}{2\hbar}\right)} \\
&= \frac{1}{\hbar}\sqrt{\frac{m}{2E}}\cot\left(\frac{\sqrt{2mE}L}{2\hbar}\right)
\end{aligned}
$$

Therefore

$$
\int_0^L dq\, G(qqE) \approx \frac{L}{\hbar}\sqrt{\frac{m}{2E}}\cot\left(\frac{\sqrt{2mE}L}{2\hbar}\right)
$$

This expression can now be expanded using the partial fraction expansion for cotangent [8]

$$
\cot(z) = \frac{1}{z} + \frac{2z}{\pi^2}\sum_{n=1}^{\infty}\left(\frac{1}{(\frac{z}{\pi})^2-n^2}\right)
$$

giving

$$
\int_0^L dq\, G(qqE) \approx \frac{L}{\hbar}\sqrt{\frac{m}{2E}}\left[\frac{2\hbar}{\sqrt{2mE}L} + \frac{\sqrt{2mE}L}{\pi^2\hbar}\sum_{n=1}^{\infty}\frac{1}{(\frac{\sqrt{2mE}L}{2\pi\hbar})^2-n^2}\right]
$$

which after further massaging gives the result stated in the main text.

[8] This standard result comes from taking the logarithm and then differentiating the infinite product formula of sine, which dates all the way back to Euler and the Basel problem [11, Chapter 9].

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