

Quantum Tunneling on Graphs

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Abstract: We explore the tunneling behavior of a quantum particle on a finite graph in the presence of an asymptotically large potential with two or three potential wells. The behavior of the particle is primarily governed by the local spectral symmetry of the graph around the wells. In the case of two wells the behavior is stable in the sense that it can be predicted from a sufficiently large neighborhood of the wells. However in the case of three wells we are able to exhibit examples where the tunneling behavior can be changed significantly by perturbing the graph arbitrarily far from the wells.

1. Introduction

Quantum tunneling is the physical phenomenon that a quantum particle can get to the other side of an energy barrier even if it is so high that this is not possible in classical mechanics. In this paper we are concerned with tunneling behavior of a non-relativistic quantum particle on a graph. The energy barrier is easiest realized by a potential that has two or more local minima, referred to as energy wells.

The motion of a non-relativistic quantum particle on a manifold is governed by the Schrödinger equation:

$$i\hbar\frac{\partial}{\partial t}\phi = H\phi.$$

Here ϕ is the quantum state of the particle, \hbar is Planck's constant and $H = -\hbar^2\Delta + V$, where Δ is the Laplace operator and V is a given potential. When the particle is started from state x , then $\phi_t(y) = K(t, x, y)$ is the propagator kernel. Its length squared, $|\phi_t(y)|^2$, is usually interpreted as the probability density that the particle is in state y at time t . According to the terminology of [6], Chap. 7, We shall refer to this as the probability of tunneling from x to y at time t .

Precise mathematical analysis of tunneling in Euclidean spaces goes back to the work of Simon ([7]) and Helffer and Sjöstrand ([4]). They investigated the time-evolution of

a wave packet concentrated primarily around one of the wells, when the height of the barrier goes to infinity, that is when $V = Q \cdot W$, where W is a fixed function and $Q \in \mathbb{R}$ is a large real number. For any fixed t the probability of such a wave packet to tunnel to the other well quickly tends to 0, this is often referred to as exponential damping in the non-relativistic case. On the other hand, for a fixed large Q , the tunneling probability may even approach 1 near time $t = \pi \exp(\sqrt{Q}\rho(x, y))$, where ρ is the so-called Agmon metric that depends only on W . This is the case for symmetric double wells studied in [7].

We shall carry out such analysis in the discrete setting. One important difference is that while in Euclidean space a particle can never be perfectly localized in a single location, the best discrete analogue of a wave packet concentrated near a well is the quantum state given by $\phi_0 = \delta_x$. Another important difference is that we do not intend to compare quantum paths to classical paths, or to talk about classical mechanics on graphs at all. Nevertheless our setup is a reasonable discretization of the smooth problem. In the smooth setup it turns out (see Theorem 2.1 in [7]) that when the potential is high enough the particle can be concentrated near one well in a sufficiently low energy state that it can not classically surmount the barrier but it can tunnel through the barrier. Thus it seems reasonable to call the discrete phenomenon “tunneling” even though we do not compare it to classical mechanics.

The Laplace operator has a natural discrete analogue on graphs and this makes it possible to define and analyze the discrete Schrödinger equation. In particular we shall recover analogues to the symmetric double well case in [7] and certain stability of this that has been observed in [8]. On the other hand we shall exhibit that such stability is no longer true when there are three wells.

Let $G(X, E)$ be a finite connected graph. For any vertex $x \in X$ we denote its degree by d_x . We think of the vertices as the possible positions of a quantum particle. At any moment t the state of the particle is given by a unit length vector $\varphi_t \in \mathbb{C}^X$, $\sum_{x \in X} |\varphi_t(x)|^2 = 1$. The quantity $|\varphi_t(x)|^2$ is interpreted as the probability of the particle being in position x . Let Δ denote the symmetrized Laplace matrix of the graph, that is

$$\Delta(x, y) = \begin{cases} 1 & \text{if } x = y \\ \frac{-1}{\sqrt{d_x d_y}} & \text{if } xy \in E \\ 0 & \text{otherwise.} \end{cases} \quad (1)$$

Remark 1. One could use the standard graph Laplacian throughout and get similar results. However one has to be careful since then neither the Hamiltonian, nor the auxiliary matrices are symmetric. This technical difficulty can be overcome by the standard method of finding symmetric conjugates. Instead we choose to work with the symmetric version of the Laplacian mainly to enhance readability.

Given a potential $V : X \rightarrow [0, \infty)$, the motion of the particle is governed by the discrete Schrödinger equation

$$-i \frac{d}{dt} \varphi_t = H \varphi_t, \quad (2)$$

where $H = \Delta - V$ is the Hamiltonian. Here and from now on we will use the same notation for a function on the set of vertices and the corresponding diagonal matrix. We want to investigate the asymptotic behavior of this quantum evolution, so we choose the potential to be $V = Q \cdot W$, where W is a fixed vector and Q is a real number going to infinity. The effect of a large Q is the same as letting $\hbar \rightarrow 0$, hence in our form the Planck’s constant is “hidden” in the potential.

Simon (see [7]) carried out asymptotic analysis of double well potentials in Euclidean space for rather general potentials. Helffer and Sjöstrand ([4], first in a series of papers) analyzed the case of multiple wells. In Sect. 1.1 we shall briefly compare our results and methods to that of Simon as there are similarities and contrasts that are worth pointing out.

We will consider potentials with two (double well) and three (triple well) global maxima. We will consider *simple potentials* meaning that the only vertices where the potential is non-zero are the wells themselves, and *general potentials*. We are primarily interested in whether tunneling takes place at all. By this we mean the following: given a large potential, will there be a time at which we can be almost sure that the particle has evolved into the other well? If not, what is the maximal probability of finding the particle in the other well? To answer these questions we introduce a new quantity we call *tunneling coefficient* to measure these probabilities asymptotically. We are also interested in around what time t does this probability become maximal. The answer to this question as a function of Q is what we call the *tunneling time*. (This is our own terminology for this conceptually simple quantity, it has nothing to do with the usual - controversial - notion of tunneling time in the physics literature.)

Definition 1. Given two states $x, y \in X$, let us start the particle in the pure state of x . We define the tunneling coefficient to be

$$\liminf_{Q \rightarrow \infty} \sup_{t \in [0, \infty)} |\varphi_t(y)|^2 = TC(x, y). \quad (3)$$

We distinguish three different behaviors: Perfect (asymptotic) tunneling happens if $TC(x, y) = 1$, partial tunneling happens if $0 < TC(x, y) < 1$ and no tunneling takes place if $TC(x, y) = 0$.

We say that the tunneling from x to y happens within $f(Q)$ time if

$$TC(x, y) = \liminf_{Q \rightarrow \infty} \sup_{t \in [0, f(Q)]} |\varphi_t(y)|^2. \quad (4)$$

Remark 2. The use of \liminf instead of \limsup in (3) and (4) is somewhat arbitrary, but it reflects our choice to emphasize the cases when there is tunneling. For example this way $TC = 1$ is a stronger statement and $TC = 0$ is seemingly weaker. However in every single case to be analyzed, the \liminf in question turns out to be a limit, so our choice makes essentially no difference.

When referring to tunneling times, apart from the standard o and O notation we will use $f = \Theta(g)$, meaning $f = O(g)$ and $g = O(f)$ at the same time.

It turns out that whether tunneling happens at all is primarily governed by the degree of similarity of the neighborhoods of the wells, and the speed of tunneling depends on the distance of the wells. More precisely:

Definition 2. Let $PR(x, k)$ denote the probability that the simple random walk started at $x \in X$ returns to x at time k . Given two vertices $x, y \in X$ we say that they are *m-cospectral* if the probability of return is the same for x and y up to time m , that is $PR(x, k) = PR(y, k)$ for every $0 \leq k \leq m$. The *cospectrality* of x and y is the maximal m for which they are *m-cospectral*. This will be denoted by $co(x, y)$.

Using this definition we can state the precise behavior of TC :

Theorem 1. *In the case of a simple double well potential where the graph-distance of the two wells x, y is denoted by $d = d(x, y)$ the following is true between x and y :*

- a) *if the two wells are d -cospectral ($co(x, y) \geq d$) then there is perfect asymptotic tunneling,*
- b) *if $co(x, y) = d - 1$ then there is partial tunneling,*
- c) *if $co(x, y) < d - 1$ then there is no tunneling.*

When there is tunneling, the tunneling time is $\Theta(Q^{d-1})$.

The triple well setup turns out to be much more complicated. To avoid excessive case analysis, here we restrict our attention to sufficiently cospectral wells. Let $x, y, z \in X$ be three points such that $a = d(x, y) \leq b = d(x, z) \leq c = d(y, z)$. Assume that the wells are pairwise c -cospectral, and let the potential be $W(x) = W(y) = W(z) = 1$ and 0 everywhere else. For any two wells u, v let us compute

$$c_{uv} = \sum_{P:u \rightarrow v, |P|=d(u,v)} \prod_{j=0}^{|P|-1} 1/\sqrt{d_{x_j} d_{x_{j+1}}}, \tag{5}$$

where $P : u \rightarrow v$ denotes any path $u = x_0, x_1, \dots, x_l = v$ in the graph and the length of this path is denoted by $|P| = l$.

Theorem 2. *With the above notation and assumptions*

- a) *If $a < b \leq c$ then there is perfect tunneling between x and y , but no tunneling to and from z . The tunneling time is $\Theta(Q^{a-1})$.*
- b) *If $a = b < c$ and the particle is started from x then it never tunnels perfectly to a single other state, but it does tunnel to a mixed state of y and z . This happens on the scale of $t \sim Q^{a-1}$.*
- c) *If $a = b < c$ and the particle is started from y , then it tunnels completely to z if and only if $c_{xy} = c_{xz}$. The tunneling time is $\Theta(Q^{a-1})$. Note that in particular, unlike in the first case, the particle can tunnel from y to z despite the fact that $d(y, x) < d(y, z)$. Comparing to the double well case, note that the speed of tunneling between y and z increased substantially after introducing the third well at x .*

The precise behavior becomes even more subtle if the wells form an equilateral triangle.

Theorem 3. *Assume $a = b = c$.*

- a) *If $c_{xy} \neq c_{xz}$ then there is only partial tunneling from y to z .*
- b) *If $c_{xy} = c_{xz}$ and $\sqrt{c_{yz}^2 + 8c_{xz}^2}$ is irrational, then there is perfect tunneling from y to z . The tunneling time f has to satisfy $Q^{a-1} = o(f(Q))$.*
- c) *If $c_{xy} = c_{xz}$ and $\sqrt{c_{yz}^2 + 8c_{xz}^2}$ is rational, then even if there is perfect tunneling from y to z , the tunneling time f has to satisfy $Q^a = O(f(Q))$. (In particular this is the case if $c_{xy} = c_{xz} = c_{yz}$.)*

Conjecture 1. *If $c_{xy} = c_{xz} \neq c_{yz}$ we believe that there is always perfect tunneling from y to z .*

In view of the characterization of the double well case, there is a very surprising instability phenomenon in the triple well case.

Theorem 4. *It is possible to construct a triple well scenario where $TC(y, z) = 4/9$, but by modifying the graph arbitrarily far from the wells only a little bit (e. g. by adding a single edge) one can achieve $TC(y, z) = 1$. Hence the tunneling coefficient is not predictable from any fixed neighborhood of the wells.*

Finally we show that tunneling can happen in the presence of more general potentials than the singular ones. In particular perfect tunneling happens in the symmetric double well case.

Theorem 5. *Let $G(X, E)$ be a graph, $x, y \in X$ and $W : X \rightarrow \mathbb{R}$ which has its global maxima in x and y . Let us further assume that there is an involutive automorphism ϕ of G that $\phi(x) = y$ and $W(\phi(v)) = W(v)$ for any vertex $v \in X$. Then there is perfect asymptotic tunneling between x and y and the tunneling time is of the usual order: $Q^{d(x,y)-1}$.*

1.1. Comparison with the results of Simon. In [7] quantum tunneling is analyzed in Euclidean space in the presence of a double well potential. More precisely Simon gives asymptotics of the eigenvalue splitting (the difference of the smallest two eigenvalues) of the Schrödinger operator H with potential $\lambda^2 V$ as $\lambda \rightarrow \infty$. As he explains in the Introduction this splitting is what determines “the time needed to evolve from a state concentrated primarily in one well into one primarily in the other”. We shall reproduce this argument in the context of graphs in the next section.

More precisely in Theorem 1.3 he proves that, for any given eigenvalue E , depending on the potential, one of three things can happen: either the corresponding eigenvector asymptotically disappears from one (or both) of the wells, or there is another eigenvalue E' very close to E . We will see that the first two cases are analogous to the case when in our Theorem 1 there is no tunneling, while the third case corresponds to partial or perfect tunneling and then according to the previous paragraph the eigenvalue splittings determine what we call the tunneling time.

Then on p. 93, [7] Simon introduces a condition on the potential referred to as (4) that, among others, ensures that in Theorem 1.3 the first two outcomes are impossible. Also on p. 93 he remarks that symmetric potentials automatically satisfy (4). Then in Theorem 1.5 he computes precise asymptotics for the eigenvalue splitting when the potential satisfies (4). Our analogue of this is Theorem 5, and though we do not formulate it in the generality as Simon does, looking at the proof of this theorem it is clear that instead of our symmetry condition we could have used a condition analogous to Simon’s (4).

As the underlying space is symmetric, the distinction between partial and perfect tunneling does not play a role in [7], and the geometry guarantees that in the case of a symmetric potential condition (4) holds so there is always perfect tunneling. On the other hand on a graph these differences do come out and the emphasis in our present paper is more on distinguishing between these general categories. In most cases the computation of the tunneling time does not require extra efforts though. This is why we introduce TC which is a convenient measure of tunneling. As it will turn out, at least in the double well case, TC depends solely on how the values of the first eigenvector are distributed among the two wells. Thus the limit value of the expression in condition (4) in [7] measures exactly the same thing (only slightly scaled), so it is directly related to our TC . In particular $TC > 0$ is equivalent to Condition (4).

Our methods also show some similarity to those of Simon: studying the heat kernel e^{-tH} associated with H one can relate the question about eigenvectors of H to sample paths of Brownian motion, or in the case of graphs, random walks.

1.2. *Intuitive explanation of tunneling.* It is easy to see that if the initial state of the particle is $\varphi = \varphi_0$ then the solution of the Schrödinger equation is given by

$$\varphi_t = e^{itH} \varphi. \tag{6}$$

This evolution (without the potential) in the context of graphs is usually referred to as the continuous time quantum walk. It has been first studied in [2]. For an overview the reader is referred to [5]. The main application of quantum walks is in quantum computing. Since the quantum walk “moves” faster than the classical random walk (see e.g. [1]) it can be used to show the power of quantum computing over classical computers.

To better understand the behavior of the solution we decompose the state-space according to eigenstates. Let $n = |X|$ denote the number of vertices of G . The matrix H is symmetric, hence it has a real spectrum with eigenvalues $\lambda_1 \leq \lambda_2 \leq \lambda_3 \leq \dots \leq \lambda_n$. Let ψ_k denote the eigenvector corresponding to the eigenvalue λ_k . Then e^{itH} has the same eigenvectors but with eigenvalues $e^{it\lambda_k}$. Thus if we write

$$\varphi = \sum_{k=1}^n c_k \psi_k, \tag{7}$$

then we get that

$$\varphi_t = \sum_{k=1}^n c_k e^{it\lambda_k} \psi_k. \tag{8}$$

If the potential well is deepest at the vertices $x, y \in X$ with value $V(x) = V(y) = Q$, then from the physical analogy one expects the two smallest (most negative) eigenvalues to be approximately $1 - Q$, and the corresponding two normalized eigenfunctions should be close to $\psi_1(x) \approx \psi_1(y) \approx \psi_2(x) \approx -\psi_2(y) \approx 1/\sqrt{2}$ and $\psi_1(z) \approx \psi_2(z) \approx 0$ if $z \in X \setminus \{x, y\}$. Then if the particle starts in x we have

$$\varphi \approx \frac{\psi_1 + \psi_2}{\sqrt{2}}. \tag{9}$$

Hence

$$\varphi_t \approx \frac{e^{it\lambda_2}}{\sqrt{2}} \left(e^{it(\lambda_1 - \lambda_2)} \psi_1 + \psi_2 \right), \tag{10}$$

so at time $t = \pi/(\lambda_1 - \lambda_2)$ the state of the particle is approximately given by $c(\psi_1 - \psi_2)$ so the particle is almost surely in state y .

In the following sections we shall make precise estimates to be able to confirm or reject the predicted behavior of the particle.

2. Asymptotics

In order to make the intuitive explanation work in reality, we have to understand asymptotic behavior of various quantities. The initial state of our particle will be $\varphi = \chi_x$, the characteristic function of the vertex $x \in X$ which is one of the vertices where the potential is minimal. Hence first of all we will be interested in the eigenvector-decomposition $\varphi = \sum_1^n c_k \psi_k$. To be able to analyze this, we will first need to understand asymptotics of the eigenvalues and eigenspaces of the Hamiltonian.

We shall always denote the increasing sequence of eigenvalues of $H = \Delta - Q \cdot W$ by $\lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_n$, and the corresponding normalized, pairwise orthogonal eigenvectors by $\psi_1, \psi_2, \dots, \psi_n$. (If there are multiple eigenvalues, the choice of ψ_i might not be unique.)

2.1. Eigenspaces. The spectrum of a matrix depends continuously on the entries. Since $H/Q = \Delta/Q - W \rightarrow -W$ if $Q \rightarrow \infty$ we can observe the following:

Claim. If the values of the unscaled potential W are $w_1 \geq w_2 \geq \dots \geq w_n$ then for all $1 \leq i \leq n$ we have

$$\lim_{Q \rightarrow \infty} \frac{\lambda_i}{Q} + w_i = 0. \quad (11)$$

Lemma 1. *For any i the eigenfunction ψ_i is asymptotically concentrated on those vertices of the graph on which the value of the unscaled potential is equal to w_i . That is $\psi_i(x) \rightarrow 0$ as $Q \rightarrow \infty$ unless $W(x) = w_i$.*

Proof. Denote by χ_x the characteristic vector of $x \in X$ and write $\chi_x = \sum c_k \psi_k$. Then $\psi_i(x) = \langle \psi_i, \chi_x \rangle = c_i$. We further have $H\chi_x = \sum \lambda_k c_k \psi_k$, and hence

$$\Delta\chi_x = (H + QW)\chi_x = H\chi_x + QW(x)\chi_x = \sum (\lambda_k + QW(x))c_k \psi_k. \quad (12)$$

Dividing both sides by Q and taking the norm-squares we get that

$$\frac{\|\Delta\|^2}{Q^2} \geq \frac{\|\Delta\chi_x\|^2}{Q^2} = \sum_{k=1}^n \left(\frac{\lambda_k}{Q} + W(x) \right)^2 c_k^2 \geq \left(\frac{\lambda_i}{Q} + W(x) \right)^2 c_i^2. \quad (13)$$

The left-hand side converges to zero, and if $W(x) \neq w_i$ then $\lambda_i/Q + W(x)$ converges to a non-zero constant, hence c_i has to converge to 0 as Q goes to infinity, and this finishes the proof. \square

A level set of the potential W is a maximal subset $L \subset X$ on which W is constant. The preceding lemma shows that for any such level set there will be precisely $|L|$ eigenfunctions of the Hamiltonian that become more and more concentrated on L , and conversely, any function concentrated on L will be more and more composed only of these $|L|$ eigenfunctions.

The ‘‘wells’’ are the vertices of the level set corresponding to the largest value of W (since we are subtracting W , this is where the potential is actually minimal). As we are interested in the behavior of a particle started from one of the wells, we need to understand the asymptotic behavior of the eigenfunctions corresponding to this level set. We know that they become concentrated on the wells and we already understand the first order behavior of the corresponding eigenvalues. However to study the tunneling phenomenon, we need a subtler description of the eigenfunctions involved to see whether tunneling actually happens or not. We also need a more precise asymptotic on the eigenvalues to be able to estimate the tunneling time.

2.2. Eigenfunctions. The method we use to understand eigenfunctions comes from the theory of random walks. It can also be thought of as the discrete analogue of the Feynman path-integral. It is well known that for any nonempty subset $L \subset X$ and a fixed function $f : L \rightarrow \mathbb{R}$ there is a unique extension $f : X \rightarrow \mathbb{R}$ that is harmonic everywhere outside of L . One possible way to do this extension is to start a random walk from a vertex x and define $f(x)$ to be the expected value of f at the point where the walk first hits L . This method can be extended to the case where we want f to be an eigenfunction of the Laplacian with eigenvalue λ outside of L . Denote the vertices of the random walk by $x = v_0, v_1, \dots, v_T$, where T is the first time when the walk enters the subset L . Then define $f(x)$ to be the expected value of $f(v_T)/(1 - \lambda)^T$. The presence of the potential makes things even more complicated, but the construction below is still inspired by the previous argument.

Let $L \subset X$ be the level set of the wells. We may assume without loss of generality that $W|_L = 1$ and $0 \leq W|_{X \setminus L} < 1$. Fix an arbitrary function $f : L \rightarrow \mathbb{R}$ and extend it to $X \setminus L$ the following way. Let us consider a walk $P = \langle x_0, x_1, \dots, x_T \rangle$ of length $|P| = T$ on the graph starting from a vertex $x = x_0 \in X$ and ending in $v = x_T \in L$ such that if $0 < j < T$ then $x_j \in X \setminus L$. Such a walk will be referred to as the walk from x to L and denoted by $P : x \rightarrow L$ or $P : x \rightarrow v$ if we want to specify the endpoint. (Thus we allow the $x \in L$ case. It is implicitly understood in the notation that the walk does not visit L except for the last vertex and maybe the first.) For any such walk P we define a weight by the formula

$$s(P) = \prod_{j=0}^{|P|-1} \frac{1}{\sqrt{d_{x_j} d_{x_{j+1}}} (1 - \lambda - QW(x_j))}. \tag{14}$$

Then we construct our extension of f using the following expression. If $x \in X \setminus L$ then put

$$f(x) = \sum_{P: x \rightarrow L} f(x_{|P|})s(P) = \sum_{v \in L} f(v) \sum_{P: x \rightarrow v} s(P). \tag{15}$$

Claim. The infinite sum $\sum_{P: x \rightarrow v} s(P)$ is absolutely convergent for large Q (and hence large λ).

Proof. Since W is strictly smaller than 1 outside of L , λ and $QW(x_j)$ can not cancel each other's effect: there are positive constants c, Q_0 such that $|1/(1 - \lambda - QW(x_j))| \leq c/Q$ for any $Q > Q_0$. Hence sorting the terms in the sum according to the length of the path P we get an upper bound in the form of a power series in c/Q . The coefficients of this power series are

$$a_k = \sum_{P: x \rightarrow v, |P|=k} \prod_{j=0}^{k-1} 1/\sqrt{d_{x_j} d_{x_{j+1}}}. \tag{16}$$

Finally to see that this power series converges it suffices to show that the a_k 's are uniformly bounded. In fact $a_k \leq \sqrt{d_x d_v}$ even if we consider all paths without any restrictions. This can be proven by induction on k as follows:

$$a_k = a_k(x) \leq \sum_{x \sim y} \frac{1}{\sqrt{d_x d_y}} a_{k-1}(y) \leq \sum_{x \sim y} \frac{\sqrt{d_y d_v}}{\sqrt{d_x d_y}} = d_x \frac{\sqrt{d_v}}{\sqrt{d_x}} = \sqrt{d_x d_v}. \tag{17}$$

This completes the proof of the claim. \square

Let us consider now a walk $P : x \rightarrow L$ and denote $y = x_1$. Let R denote the walk y, x_2, \dots, x_T , i. e. R is obtained from P by removing the first vertex, and $P = xR$. By definition $s(R) = s(P)\sqrt{d_x d_y}(1 - \lambda - QW(x))$, and obviously $|R| = |P| - 1$. Thus we can partition all paths $P : x \rightarrow L$ according to their second vertex (denoted by x_1) to arrive at the following identity:

$$\begin{aligned} f(x) &= \sum_{xy \in E} \sum_{R: y \rightarrow L} f(x_{|R|+1})s(xR) \\ &= \frac{1}{1 - \lambda - QW(x)} \sum_{xy \in E} \frac{1}{\sqrt{d_x d_y}} \sum_{R: y \rightarrow L} f(x_{|R|+1})s(R) \\ &= \frac{1}{1 - \lambda - QW(x)} \sum_{xy \in E} \frac{f(y)}{\sqrt{d_x d_y}}. \end{aligned} \quad (18)$$

Multiplying both sides by $1 - \lambda - QW(x)$ we see that $(Hf)(x) = \lambda f(x)$, hence f behaves like an eigenfunction of the Hamiltonian for every vertex in $X \setminus L$. We could actually use the same formula to “extend” f to L , only it is already defined there. Hence the condition that f is really an eigenfunction for H is equivalent to saying that the “extension” agrees with the starting value. Hence for every $v \in L$ we get an equation

$$f(v) = \sum_{P: v \rightarrow L} f(x_T)s(P) = \sum_{w \in L} f(w) \sum_{P: v \rightarrow w} s(P). \quad (19)$$

Let us denote by $Z_{vw}(\lambda, Q) = \sum_{P: v \rightarrow w} s(P)$ the sum of the weights for all paths from v to w , as a function of λ and Q . (We are still only considering paths that do not visit L except for maybe the two endpoints. In particular this definition also makes sense in the case when there are adjacent vertices in L .) These functions form an $|L| \times |L|$ symmetric, real matrix $Z = (Z_{vw})$ and the conditions on the values $f|_L$ can be written simply as $f|_L = Z \cdot f|_L$. This is analogous to the “interaction matrix” of [4]. Hence we have reduced the problem of analyzing eigenfunctions of an $n \times n$ matrix to understanding eigenfunctions of an $|L| \times |L|$ symmetric matrix whose entries are real valued functions. This isn’t a huge gain in general, but for the particular cases we are interested in, it does help a lot, as we shall see.

2.3. Symmetric double wells – the proof of Theorem 5. To illustrate the usefulness of the matrix $Z(\lambda, Q)$ we investigate the case when W has 2 global maxima: x and y , and there is an involution of G exchanging x and y that preserves W . The involution induces a bijection between paths from x to x and paths from y to y . Also there is a bijection between paths from x to y and paths from y to x . These bijections obviously preserve the weight $s(P)$. Hence $Z_{xx} = Z_{yy}$ and $Z_{xy} = Z_{yx}$. This way the eigenvectors of the matrix Z are automatically $(1, 1)$ and $(1, -1)$ with respective eigenvalues $Z_{xx} \pm Z_{xy}$. This means that the eigenvectors for H are exactly as we have presumed in Sect. 1.2. Hence there is perfect asymptotic tunneling, exactly as described there. To determine the tunneling time we need to understand that for fixed Q , how the solutions of $Z_{xx}(\lambda_1, Q) + Z_{xy}(\lambda_1, Q) = 1$ and $Z_{xx}(\lambda_2, Q) - Z_{xy}(\lambda_2, Q) = 1$ relate to each other. Let us introduce the auxiliary variable $h = (1 - \lambda)/Q$. Now the weight of each path can be rewritten as

$$s(P) = \frac{1}{Q^{|P|}} \prod_{j=0}^{|P|-1} \frac{1}{\sqrt{d_{x_j} d_{x_{j+1}}} (h - W(x_j))}. \quad (20)$$

Let us write $s'_P = s'_P(h) = s(P)(h-1)Q^{|P|}$. Then, since we know that $h \rightarrow 1$ as $Q \rightarrow \infty$ and that $0 \leq W(v) < 1$ when v is not a well, we get that s'_P tends to some constant as $h \rightarrow 1$. Now, after multiplying by $h-1$, the equations for the eigenvalues of Z being equal to 1 can be written as

$$h-1 = \sum_{P:x \rightarrow x} \frac{s'_P(h)}{Q^{|P|}} \pm \sum_{P:x \rightarrow y} \frac{s'_P(h)}{Q^{|P|}}. \quad (21)$$

Denoting the solutions of each version by h_1, h_2 , taking the difference of the two equations and dividing by $h_1 - h_2$ we get

$$1 = \sum_{P:x \rightarrow x} \frac{s'_P(h_1) - s'_P(h_2)}{(h_1 - h_2)Q^{|P|}} + \frac{Q^{-d(x,y)}}{h_1 - h_2} \sum_{P:x \rightarrow y} \frac{s'_P(h_1) + s'_P(h_2)}{Q^{|P|-d}}. \quad (22)$$

Since each s'_P is clearly differentiable and the length of any $x \rightarrow x$ path is at least 2 by definition, the first sum on the right hand side goes to 0 as $Q \rightarrow \infty$. In the second sum all the s'_P 's converge to some constants, and hence all terms where $|P| > d(x, y)$ go to 0, while those finitely many terms where $|P| = d(x, y)$ converge to constants. Hence $Q^{-d(x,y)}/(h_1 - h_2)$ has to converge to a constant too. Thus we get $h_1 - h_2 \sim 1/Q^{d(x,y)}$ and hence $\lambda_1 - \lambda_2 \sim 1/Q^{d(x,y)-1}$. Combining this with the observations in Sect. 1.2 we get that the tunneling time is of order $Q^{d(x,y)-1}$. \square

3. Simple Potential

In this section we are going to analyze the two and three well scenarios where the potential wells are ‘‘singular’’, in the sense that $W(v) = 0$ if v is not one of the wells and $W(v) = 1$ at each well. In this case the entries of matrix Z have particularly simple dependence on Q which makes the analysis possible. First of all, the weight function on paths becomes

$$s(P) = \frac{1}{(1-\lambda)^{|P|}} \prod_{j=0}^{|P|-1} \frac{1}{\sqrt{d_{x_j} d_{x_{j+1}}}}, \quad (23)$$

when the starting vertex of P is not a well. For paths starting from the wells we get

$$s(P) = \frac{1-\lambda}{1-\lambda-Q} \frac{1}{(1-\lambda)^{|P|}} \prod_{j=0}^{|P|-1} \frac{1}{\sqrt{d_{x_j} d_{x_{j+1}}}}. \quad (24)$$

This finally gives

$$Z_{vw}(\lambda, Q) = \frac{1-\lambda}{1-\lambda-Q} \sum_{k=1}^{\infty} \frac{1}{(1-\lambda)^k} \sum_{\substack{P:v \rightarrow w \\ |P|=k}} \prod_{j=0}^{k-1} \frac{1}{\sqrt{d_{x_j} d_{x_{j+1}}}}. \quad (25)$$

The last part of the formula is independent of λ and Q . Hence we can introduce the notation

$$P_{vw}(k) = \sum_{\substack{P:v \rightarrow w \\ |P|=k}} \prod_{j=0}^{k-1} \frac{1}{\sqrt{d_{x_j} d_{x_{j+1}}}}, \quad (26)$$

so we have

$$Z_{vw}(\lambda, Q) = \frac{1 - \lambda}{1 - \lambda - Q} \sum_{k=1}^{\infty} \frac{P_{vw}(k)}{(1 - \lambda)^k}. \quad (27)$$

Claim. For any $x \in X$ the value of $P_{xx}(k) = PR(x, k)$ is exactly the probability that the simple random walk which started from x returns after k steps.

Proof. For any closed path $P : x = x_0, x_1, \dots, x_T = x$ since the starting and endpoint are the same, we actually have

$$\prod_{j=0}^{T-1} \frac{1}{\sqrt{d_{x_j} d_{x_{j+1}}}} = \prod_{j=0}^{T-1} \frac{1}{d_{x_j}}, \quad (28)$$

and this is exactly the probability of the random walk traversing P . Hence the sum for all P of length k is exactly the probability of return in k steps. \square

We are interested in when 1 is an eigenvalue of the matrix $Z(\lambda, Q) = (Z_{vw}(\lambda, Q))$, but this is clearly equivalent to $(1 - \lambda - Q)/(1 - \lambda) = 1 - Q/(1 - \lambda)$ being an eigenvalue of the transformed matrix $\tilde{Z}(\lambda)$ which consists of entries

$$(\tilde{Z})_{vw} = \sum_{k=1}^{\infty} \frac{P_{vw}(k)}{(1 - \lambda)^k}. \quad (29)$$

Summarizing what we have computed until now: if Q is large, then the Hamiltonian will have two eigenvalues close to $-Q$. The corresponding eigenfunctions restricted to the wells will be eigenfunctions of the matrix \tilde{Z} with eigenvalue $1 - Q/(1 - \lambda)$. On the other hand if you start with an eigenfunction of \tilde{Z} with eigenvalue $1 - Q/(1 - \lambda)$ then extending it by formula (15) we get an eigenfunction of H with eigenvalue λ . We are in very good shape now, as for any eigenfunction of $\tilde{Z}(\lambda)$ there is a unique Q that makes it into an eigenfunction with eigenvalue $1 - Q/(1 - \lambda)$ and the preceding argument ensures that $Q \approx -\lambda$ if λ is large enough. This way we can get rid of the Q parameter and only work with $\tilde{Z}(\lambda)$. This matrix is symmetric, since for any path $P : v \rightarrow w$ the reverse \bar{P} is a path from w to v with the same length and weight (the latter is so because we are using the symmetrized Laplacian).

3.1. Double wells – the proof of Theorem 1. Let us start with the classical case, when there are two wells, x and y and the matrix $\tilde{Z}(\lambda)$ is 2×2 . The first question we have to answer is whether there is tunneling or not. This depends on how the two eigenvectors of $\tilde{Z}(\lambda)$ behave. Let us denote the two coordinates of an eigenvector by $f_\lambda(x)$ and $f_\lambda(y)$, noting the dependence on λ . Since $\tilde{Z}_{xy}(\lambda) \neq 0$, neither coordinates of the eigenvector will be zero. Thus in both equations coming from (19) we can divide by term on the left hand side and combine the two equations into one, obtaining

$$\tilde{Z}_{xx}(\lambda) + \frac{f_\lambda(y)}{f_\lambda(x)} \tilde{Z}_{xy}(\lambda) = \frac{f_\lambda(x)}{f_\lambda(y)} \tilde{Z}_{yx}(\lambda) + \tilde{Z}_{yy}(\lambda). \quad (30)$$

Using the symmetry of \tilde{Z} and putting $\alpha = \alpha(f) = f_\lambda(x)/f_\lambda(y)$ we get

$$\tilde{Z}_{xy} \left(\alpha - \frac{1}{\alpha} \right) = \tilde{Z}_{xx} - \tilde{Z}_{yy}. \quad (31)$$

Since our eigenvectors are normalized, we are only interested in the limiting behavior of α as $\lambda \rightarrow -\infty$. Since there are two eigenvectors and they are orthogonal, if the other eigenvector is g then $\alpha(g) = -1/\alpha(f)$. Hence the limiting behavior of $\alpha(f)$ and $\alpha(g)$ together as an unordered pair is clearly determined by the behavior of $\alpha - 1/\alpha$. Hence the only thing we have to understand is

$$\lim_{\lambda \rightarrow -\infty} \left(\alpha - \frac{1}{\alpha} \right) = \lim_{\lambda \rightarrow -\infty} \frac{\tilde{Z}_{xx}(\lambda) - \tilde{Z}_{yy}(\lambda)}{\tilde{Z}_{xy}(\lambda)}. \quad (32)$$

Further simplifying notation by writing $t = 1/(1 - \lambda)$ we have to analyze the limit

$$\lim_{t \rightarrow +0} \frac{\sum_{k=2}^{\infty} (P_{xx}(k) - P_{yy}(k))t^k}{\sum_{k=1}^{\infty} P_{xy}(k)t^k}. \quad (33)$$

The denominator's leading term is clearly $t^{d(x,y)}$, where $d(x, y)$ denotes the distance between x and y in the graph. Depending on the graph, three different limiting behaviors are possible. If for some $k < d(x, y)$ the difference $P_{xx}(k) - P_{yy}(k)$ is non-zero (i.e. the cospectrality of the wells is less than $d - 1$), then the limit will be $\pm\infty$, hence the two eigenvectors tend to $(0, 1)$ and $(1, 0)$. In this case the initial state of the particle is almost an eigenstate itself, so the particle will remain very close to its initial state, there is no asymptotic tunneling at all.

If for all $k \leq d(x, y)$ the difference $P_{xx}(k) - P_{yy}(k)$ is zero (i. e. when the wells are d -cospectral), then the limit is 0, hence the two eigenvectors tend to $(1/\sqrt{2}, 1/\sqrt{2})$ and $(1/\sqrt{2}, -1/\sqrt{2})$. This is exactly the setting of Sect. 1.2. As we have seen in Sect. 2.1 all but two c_k 's in (7) converge to 0, and we have just shown that the remaining two converge to the same value $1/\sqrt{2}$. Hence according to the argument in Sect. 1.2 the tunneling is asymptotically perfect between x and y .

Finally in the case when the first non-zero difference $P_{xx}(k) - P_{yy}(k)$ is for $k = d(x, y)$, that is, the cospectrality of the wells is exactly $d - 1$, the limit will be a non-zero constant $c = (P_{xx}(d(x, y)) - P_{yy}(d(x, y)))/P_{xy}(d(x, y))$. Hence the two eigenvectors will converge to (a, b) and $(-b, a)$, where $a/b - b/a = c$, $a^2 + b^2 = 1$. In this case $a \neq b$ and in (7) the two non-vanishing coefficients stabilize to a and $-b$. Hence we get

$$\varphi_t(x) \approx e^{it\lambda_2} \left(e^{it(\lambda_1 - \lambda_2)} a^2 + b^2 \right).$$

So maximal tunneling still occurs at time $t = \pi/(\lambda_1 - \lambda_2)$, however it is not perfect tunneling. The probability of the state x never goes asymptotically below b^2 , and the probability of the state y never goes above $a^2 = 1 - b^2$.

To finish the proof of Theorem 1 we have to estimate the tunneling time. From the arguments in Sect. 1.2 it is clear that the tunneling time is approximately $\pi/|\lambda_1 - \lambda_2|$, where λ_1 and λ_2 are the eigenvalues corresponding to the two eigenfunctions concentrated on the wells. The difficulty is that until this point we “fixed” λ , and chose an eigenvector for $\tilde{Z}(\lambda)$. We didn't have to worry about the eigenvalue, because we could always find a suitable Q for which everything worked in the end. Of course since \tilde{Z}

has two eigenvalues, we actually get two choices for Q , each of which gives one of the eigenvectors in return. Now we have to reverse things, and compute the two possible λ 's as a function of Q . To do this, first we describe how the two possible Q 's behave as the function of λ .

Let $\nu_{1,2}$ denote the two eigenvalues of \tilde{Z} . Then, since $\nu = 1 - Q/(1 - \lambda)$ has to hold, the possible choices for Q are given by $Q_{1,2} = (1 - \lambda)(1 - \nu_{1,2})$. The $\nu_{1,2}$ are given as the solution of a quadratic polynomial, so we can write them down explicitly:

$$\nu_{1,2} = \frac{\tilde{Z}_{xx} + \tilde{Z}_{yy} \pm \sqrt{(\tilde{Z}_{xx} - \tilde{Z}_{yy})^2 + (2\tilde{Z}_{xy})^2}}{2}, \tag{34}$$

hence both roots are real and we can compute:

$$h(\lambda) = Q_1 - Q_2 = (1 - \lambda) \left(\sqrt{(\tilde{Z}_{xx} - \tilde{Z}_{yy})^2 + (2\tilde{Z}_{xy})^2} \right). \tag{35}$$

We have already seen that Q_1 is a power series of the form $Q_1(\lambda) = \lambda + c_0 + c_1/\lambda + c_2/\lambda^2 + \dots$, and by the definition of h we have $Q_2(\lambda) = Q_1(\lambda) - h(\lambda)$. Let us denote the inverses of $Q_1(\lambda)$ and $Q_2(\lambda)$ by $\lambda_1(Q)$ and $\lambda_2(Q)$. We will see that $h(\lambda)$ is a power series in $1/\lambda$ with no constant term and then by the following lemma we get that $\lambda_2(Q) - \lambda_1(Q) = h(Q) + o(h(Q))$, so the tunneling time turns out to be $\pi/(h(Q) + o(h(Q)))$.

Lemma 2. *Let $f(t) = t + c_0 + c_1/t + c_2/t^2 + \dots$, and let $g(t) = f(t) - h(t)$, where $h(t)$ is a power series in $1/t$ with no constant term. Then $g^{-1}(t) = f^{-1}(t) + h(t) + o(h(t))$.*

Proof. $g^{-1}(t) = f^{-1}(f(g^{-1}(t))) = f^{-1}(g(g^{-1}(t)) + h(g^{-1}(t))) = f^{-1}(t + h(g^{-1}(t))) = f^{-1}(t) + f^{-1'}(t)h(g^{-1}(t)) + o(h(g^{-1}(t)))$. But $f^{-1'}(t) = 1 + o(1)$ and $g^{-1}(t) = t + O(1)$, hence $h(g^{-1}(t)) = h(t + O(1)) = h(t) + o(h(t))$. Putting these together we see that indeed $g^{-1}(t) = f^{-1}(t) + h(t) + o(h(t))$.

It can be seen from (35) that the order of magnitude of $h(\lambda)$ is the larger of the magnitudes of $\tilde{Z}_{xx} - \tilde{Z}_{yy}$ and of \tilde{Z}_{xy} . The latter is always $1/\lambda^{d(x,y)}$, while the former is by definition $1/\lambda^{co(x,y)+1}$. There is tunneling only if $co(x, y) + 1 \geq d$, hence the magnitude of h is always governed by the $1/\lambda^d$ term, hence the magnitude of the tunneling time is $1/h(Q) \approx Q^{d(x,y)-1}$, as claimed. \square

3.2. Triple wells. Let now the three wells be denoted by x, y, z . This time we have to analyze the eigenfunctions of a 3-by-3 matrix $\tilde{Z}(\lambda)$ instead of a 2-by-2. Let us denote the pairwise distances between the wells by $a = d(x, y) \leq b = d(x, z) \leq c = d(y, z)$. Henceforth we shall assume that the wells are pairwise $2a$ -cospectral. Though the general case could be done along the same lines, we confine ourselves to the study of sufficiently cospectral wells, mainly in order to reduce the number of cases to check. Already in this special case we are able to exhibit interesting phenomena. As we shall see, there are different types of behaviors depending on the distances between the wells: (i) $a < b \leq c$, (ii) $a = b < c$, (iii) $a = b = c$. Before looking at the particular cases, we can further simplify the matrix \tilde{Z} a little.

If we subtract $\tilde{Z}_{xx}(\lambda)$ from each diagonal entry in \tilde{Z} then we only change the eigenvalues, but not the eigenvectors of the matrix. By the cospectrality assumption

$\tilde{Z}_{yy} - \tilde{Z}_{xx} = O(1/(1-\lambda)^{2a}) = \tilde{Z}_{zz} - \tilde{Z}_{xx}$. The modified matrix for the triple well case looks like this (remembering that $a \leq b \leq c$):

$$\tilde{Z} - \tilde{Z}_{xx}I = \frac{1}{(1-\lambda)^a} \cdot \begin{pmatrix} 0 & f_0(\lambda) & f_{b-a}(\lambda) \\ f_0(\lambda) & f_{a+a'}(\lambda) & f_{c-a}(\lambda) \\ f_{b-a}(\lambda) & f_{c-a}(\lambda) & f_{a+a''}(\lambda) \end{pmatrix}, \quad (36)$$

where $a', a'' \geq 0$ and each entry denotes a power series, the index indicating the first term that may have non-zero coefficient: $f_m(t) = \sum_{k=m}^{\infty} c_k/(1-\lambda)^k$, such that $c_m \neq 0$. By abuse of notation, even if there are equalities among the indices, the corresponding power series are allowed to be different. For large λ the eigenvalues and eigenvectors of this matrix can be approximated by taking the limit of the matrix on the right-hand side. Let

$$M = \lim_{\lambda \rightarrow \infty} \begin{pmatrix} 0 & f_0(\lambda) & f_{b-a}(\lambda) \\ f_0(\lambda) & f_{a+a'}(\lambda) & f_{c-a}(\lambda) \\ f_{b-a}(\lambda) & f_{c-a}(\lambda) & f_{a+a''}(\lambda) \end{pmatrix} \quad (37)$$

denote the limit of this matrix as $\lambda \rightarrow \infty$. Note that M depends only on the graph and the position of the wells.

Definition 3. We say that the system given by the three wells in the graph is well-behaved if for large Q the three eigenvectors of \tilde{Z} are distinct and converge to three distinct limiting vectors as Q goes to infinity. These vectors then have to form an eigenbasis of M . Let ψ_1, ψ_2, ψ_3 denote the three limit vectors and μ_1, μ_2, μ_3 denote the corresponding eigenvalues of M .

Remark 3. If M has three distinct eigenvalues then the system is automatically well-behaved.

Lemma 3. Assume that the system is well-behaved. Then a necessary condition for perfect asymptotic tunneling from y to z is that $\psi_3(x) = \psi_3(y) + \psi_3(z) = 0 = \psi_1(y) - \psi_1(z) = \psi_2(y) - \psi_2(z)$ for some permutation of the eigenvectors.

Proof. Assume that there is perfect asymptotic tunneling from y to z . Since the system is well-behaved, the three relevant eigenvectors of the Hamiltonian restricted to the wells converge to three well-defined eigendirections of M . Using the definition of perfect tunneling and compactness, it is easy to see that we get three real numbers r_1, r_2, r_3 and three unit complex numbers ρ_1, ρ_2, ρ_3 such that $(0, 1, 0) = \sum r_j \psi_j$ and $(0, 0, 1) = \sum \rho_j r_j \psi_j$.

If either of the r_j 's would be 0, then (assuming r_1 is zero) we get that $(0, \rho_2, -1) = (\rho_2 - \rho_3)r_3\psi_3$. Since ψ_3 is real, this can only be if $\rho_2 = \pm 1$. Since obviously $\rho_3 \neq \rho_2$ we may assume wlog that $\rho_2 \neq -1$, hence $\rho_2 = 1$ and $\psi_3 = c(0, 1, -1)$. This proves the part of the statement involving ψ_3 , the rest follows by orthogonality of the eigenvectors.

Now we assume neither of the r_j 's is 0, and denote $\Psi_j = r_j \psi_j$. Next we show that $\Psi_j(x)$ has to be 0 for at least one j . Assume this is not true. Then $\sum \Psi_j(x) = 0$ and $\sum \rho_j \Psi_j(x) = 0$. From this we get that $(\rho_1 - \rho_2)\Psi_2(x) + (\rho_1 - \rho_3)\Psi_3(x) = 0$. Since none of the $\Psi_j(x)$'s are zero, this implies that ρ_1 is a convex combination of ρ_2 and ρ_3 . For unit complex numbers this can only be if they are all equal – a contradiction.

So we may assume $\Psi_3(x) = \psi_3(x) = 0$. But then $\Psi_1(x) = -\Psi_2(x) \neq 0$ and $\rho_1 \Psi_1(x) = -\rho_2 \Psi_2(x)$, hence $\rho_1 = \rho_2$. Looking at y we get that $\Psi_1(y) + \Psi_2(y) + \Psi_3(y) =$

1, while $\rho_1(\Psi_1(y) + \Psi_2(y)) + \rho_3\Psi_3(y) = 0$. This can only happen if $\rho_1 = -\rho_3 = \pm 1$. We may again wlog assume that $\rho_1 = 1$ and $\rho_3 = -1$. Finally taking the difference $(0, 1 - 1) = (0, 1, 0) - (0, 0, 1) = 2r_3\psi_3$, we get that $\psi_3(z) + \psi_3(y) = 0$. The rest of the statement follows from orthogonality again. \square

Whether the above condition is also sufficient for perfect tunneling is described in the next lemma.

Lemma 4. *Assume that the system is well-behaved, not all eigenvalues of M are the same, $\psi_3(x) = \psi_3(y) + \psi_3(z) = 0$ and that neither $\psi_1(x)$ nor $\psi_2(x)$ is 0. Let*

$$\gamma = \frac{\mu_1 - \mu_3}{\mu_1 - \mu_2}. \quad (38)$$

- If $\gamma = p/q$ is rational where $p \in \mathbb{Z}$ is odd while $q \in \mathbb{Z}$ is even, then there is perfect tunneling from y to z in time $O(Q^{a-1})$. This also includes the case when $\gamma = \infty$.*
- If γ is irrational, then there is perfect tunneling from y to z , but the tunneling time f has to satisfy $Q^{a-1} = o(f(Q))$.*
- Otherwise we cannot say for sure that there is perfect tunneling from y to z . However if there is, the tunneling time f has to satisfy $Q^a = O(f(Q))$.*

Proof. Let ν be an eigenvalue of \tilde{Z} with eigenvector ψ . Let us recall that ψ is the restriction of an eigenfunction of the Hamiltonian to the wells with eigenvalue λ if and only if $Q = (1 - \lambda)(1 - \nu)$. If we denote by $\nu_j = \nu_j(\lambda) : j = 1, 2, 3$ the eigenvalues of the matrix on the right-hand side of (36) then on one hand $\mu_j = \lim_{\lambda \rightarrow \infty} \nu_j$, on the other hand the eigenvalues of \tilde{Z} are $\nu_j/(1 - \lambda)^a + \tilde{Z}_{xx}(\lambda)$ and the solutions for Q are given by

$$Q_j = (1 - \lambda)(1 - \tilde{Z}_{xx}(\lambda) - \nu_j/(1 - \lambda)^{a-1}) : j = 1, 2, 3. \quad (39)$$

Denoting the inverse functions by $\lambda_j(Q) : j = 1, 2, 3$ we see that the three relevant eigenvalues of the Hamiltonian are precisely the $\lambda_j(Q)$'s.

Since $\psi_1(x)$ and $\psi_2(x)$ are non-zero, all three eigenvectors participate in the decomposition of the pure state y . Then from the proof of the previous lemma we can see that perfect tunneling takes place from y to z in time $f(Q)$ if and only if for large Q there is a $t \in [0, f(Q)]$ and a unit complex number ρ such that $e^{it\lambda_1(Q)} \approx e^{it\lambda_2(Q)} \approx \rho$ and $e^{it\lambda_3(Q)} \approx -\rho$. (Here $\lambda_3(Q)$ corresponds to the eigenvector ψ_3 in the previous proof.) More precisely when

$$\limsup_{Q \rightarrow \infty} \inf_{t \in [0, f(Q)]} |e^{it(\lambda_1(Q) - \lambda_2(Q))} - 1|^2 + |e^{it(\lambda_1(Q) - \lambda_3(Q))} + 1|^2 = 0. \quad (40)$$

Let us introduce the lattice $\mathcal{L} = \{(p, q) \in \mathbb{Z}^2 : p \equiv 0(2), q \equiv 1(2)\}$ and denote by

$$\Gamma = \left\{ \left(t \frac{\lambda_1(Q) - \lambda_2(Q)}{\pi}, t \frac{\lambda_1(Q) - \lambda_3(Q)}{\pi} \right) \in \mathbb{R}^2 : t \in [0, f(Q)] \right\}, \quad (41)$$

the relevant curve traced out in \mathbb{R}^2 as t runs over the interval $[0, f(Q)]$. Then (40) is equivalent to

$$\limsup_{Q \rightarrow \infty} \text{dist}(\mathcal{L}, \Gamma) = 0. \quad (42)$$

Let us analyze what happens to the curve Γ as $Q \rightarrow \infty$. Using (39) together with Lemma 2 we can write

$$\lambda_{j_1}(Q) - \lambda_{j_2}(Q) = (1 + O(1/Q))(v_{j_1}(Q) - v_{j_2}(Q))/(1 - Q)^{a-1}. \quad (43)$$

If $f(Q) = o(Q^a)$, then clearly Γ converges uniformly to a segment through the origin whose slope is γ and whose length is of magnitude $f(Q)/Q^{a-1}$. First of all, if $f(Q) = o(Q^{a-1})$ then Γ converges uniformly to a single point, namely the origin. As $(0, 0) \notin \mathcal{L}$, in this case there can not be perfect tunneling.

- a) If $\gamma = q/p$ is rational where $q \in \mathbb{Z}$ is odd while $p \in \mathbb{Z}$ is even, then the line with slope γ passes through a point of \mathcal{L} . Hence there is a constant K such that if $f(Q) = KQ^{a-1}$ then the limit segment of Γ will pass through \mathcal{L} , hence (42) will hold. Thus there is perfect tunneling in time $O(Q^{a-1})$.
- b) If γ is irrational, then the line of slope γ will pass arbitrarily close to \mathcal{L} . If $f(Q) = O(Q^{a-1})$, then the length of the limiting segment will be bounded, hence the lim sup in (42) will be strictly positive and there will not be perfect tunneling. On the other hand if $Q^{a-1} = o(f(Q))$, then Γ will arbitrarily approximate any finite piece of the limiting line, hence there will be perfect asymptotic tunneling.
- c) Finally, if γ is rational but not odd-over-even, then the lattice will be separated from the limiting line. Hence if $f(Q) = o(Q^a)$, then the lim sup in (42) will be positive again. Thus tunneling cannot take place within time $o(Q^a)$. \square

Lemma 5. *If the slope of Γ , that is $(\lambda_1(Q) - \lambda_3(Q))/(\lambda_1(Q) - \lambda_2(Q))$, is not a constant as a function of Q , then in case c) of the previous lemma there is perfect tunneling. On the other hand if this is a constant function and γ is rational but not odd-over-even, then there is no perfect tunneling at all.*

Proof. It is clear that if $(\lambda_1(Q) - \lambda_3(Q))/(\lambda_1(Q) - \lambda_2(Q))$ is constant (and thus equal to γ which is not odd-over-even), then even with the choice of $f(Q) = \infty$ the distance between the line Γ and the lattice \mathcal{L} will be positive, hence tunneling can not take place.

If $\gamma(Q) = (\lambda_1(Q) - \lambda_3(Q))/(\lambda_1(Q) - \lambda_2(Q))$ is non-constant, then it is an analytic function (since it is given by a convergent Taylor series) converging to γ as Q goes to infinity. In particular there is a Q_0 such that if $Q > Q_0$, then $\gamma \neq \gamma(Q)$. For any fixed Q if $\gamma(Q)$ is irrational, then $\text{dist}(\mathcal{L}, \Gamma) = 0$. On the other hand if $\gamma(Q) = r/s$ for some integers r, s , then letting time go to infinity (that is, choosing $f(Q) = \infty$) it is easy to see by elementary number theory that $\text{dist}(\mathcal{L}, \Gamma) \leq 1/s$. Since $\gamma(Q) \rightarrow \gamma$ this means (using that $\gamma(Q)$ is actually different from γ !) that $s \rightarrow \infty$, hence $\limsup_{Q \rightarrow \infty} \text{dist}(\mathcal{L}, \Gamma) = 0$. This finishes the proof of the lemma. \square

Proof (Proof of Theorem 2). We have to consider two cases:

$a < b \leq c$:. In this case

$$M = \begin{pmatrix} 0 & c_1 & 0 \\ c_1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad (44)$$

hence the eigenvectors of \tilde{Z} converge to $(1, 1, 0)/\sqrt{2}$; $(1, -1, 0)/\sqrt{2}$; $(0, 0, 1)$ with respective eigenvalues $c_1, -c_1, 0$. This of course means that there is complete asymptotic tunneling between the two nearest wells, and there is no tunneling to or from the third well. Further we get that the tunneling time is asymptotically $\pi/|\lambda_1(Q) - \lambda_2(Q)| = \pi(1 - Q)^{a-1}/(2c_1)$.

$a = b < c$ ∴ In this case

$$M = \begin{pmatrix} 0 & c_1 & c_2 \\ c_1 & 0 & 0 \\ c_2 & 0 & 0 \end{pmatrix}. \quad (45)$$

Let us denote $r = \sqrt{c_1^2 + c_2^2}$. Then M 's eigenvectors are

$$\begin{aligned} \psi_1 &= \frac{(-r, c_1, c_2)}{\sqrt{2}r}, \\ \psi_2 &= \frac{(r, c_1, c_2)}{\sqrt{2}r}, \\ \psi_3 &= \frac{(0, -c_2, c_1)}{r}. \end{aligned} \quad (46)$$

The corresponding eigenvalues are $-r$, r and 0 , hence the system is well-behaved. Some computation from (36) shows that $v_1(\lambda) \sim 1/(1-\lambda)^{c-a}$. So if the particle starts from state x then, since $(1, 0, 0)$ is a multiple of $(\psi_2 - \psi_1)$, we get that the particle tunnels to the mixed state in which the probability of being in y and z is both $1/2$.

The situation is different if we start the particle from y . By Lemma 3 it follows that if $c_1 \neq c_2$ then there cannot be complete tunneling from y to z . So let us assume $c_1 = c_2$. Since $r \neq 0$, all conditions of Lemma 4 are satisfied and $|\gamma| = 1/2$, hence part a) applies and we get that there is perfect tunneling in time $\Theta(Q^{a-1})$. \square

3.3. Equilateral triple wells. We are still using all the above notations, in particular we are analyzing \tilde{Z} using (36). Now we have

$$M = \begin{pmatrix} 0 & c_{xy} & c_{xz} \\ c_{xy} & 0 & c_{yz} \\ c_{xz} & c_{yz} & 0 \end{pmatrix}, \quad (47)$$

where the c 's are defined according to (5) and depend on the particular geodesics connecting the wells.

Proof (Proof of Theorem 3). All of the c 's are strictly positive, hence M has no eigenvectors with a single non-zero entry. This implies that some partial tunneling always happens. The question is how to determine when perfect tunneling happens. It is easy to see that M is non-singular, hence its eigenvalues are non-zero reals. The characteristic polynomial is $x^3 - (c_{xy}^2 + c_{xz}^2 + c_{yz}^2)x - 2c_{xy}c_{xz}c_{yz}$. If this has multiple roots then it has a common root with its derivative and just looking at the signs, this common root can only be $x = -\sqrt{(c_{xy}^2 + c_{xz}^2 + c_{yz}^2)}/3$. But that implies $\sqrt[3]{c_{xy}c_{xz}c_{yz}} = \sqrt{c_{xy}^2 + c_{xz}^2 + c_{yz}^2}/3$, which can only happen if $c_{xy} = c_{xz} = c_{yz}$ since the c 's are non-negative.

Let us first assume this is not the case. Then there are no multiple eigenvalues hence the system is well-behaved. Thus there are three distinct eigenvectors, which are the limits of the corresponding eigenvectors of the right-hand side of (36). As before, we denote the three eigenvectors by ψ_1, ψ_2, ψ_3 .

Clearly, the condition of Lemma 3 for ψ_3 is equivalent to $c_{xy} = c_{xz}$. This proves part a) of the theorem. It is also not difficult to compute that the eigenvalues are $\mu_{1,2} = \frac{c_{yz} \pm \sqrt{c_{yz}^2 + 8c_{xz}^2}}{2}$, $\mu_3 = -c_{yz}$. Thus in this case

$$\gamma = \frac{3c_{yz} + \sqrt{c_{yz}^2 + 8c_{xz}^2}}{2\sqrt{c_{yz}^2 + 8c_{xz}^2}}. \quad (48)$$

Since the c 's are rational numbers by construction, γ is rational if and only if $\sqrt{c_{yz}^2 + 8c_{xz}^2}$ is rational. \square

Claim. If γ is rational it cannot be odd-over-even.

Proof. By multiplying through with the appropriate integer, we may assume that c_{yz} , c_{xz} are coprime integers. If c_{yz} is odd then so is $\sqrt{c_{yz}^2 + 8c_{xz}^2}$, hence the numerator is even and the denominator is twice an odd number, hence γ cannot be odd-over-even. So we may assume $c_{yz} = 2p$, hence c_{xz} is odd (as they are coprime). But then $2\sqrt{p^2 + 2c_{xz}^2}$ cannot be an integer, since $p^2 + 2c_{xz}^2$ is 2 or 3 modulo 4, which means it cannot be a full square. This is a contradiction hence the claim is true. \square

Lemma 4 now implies parts b) and c) of the theorem, except for the case when $c_{xy} = c_{xz} = c_{yz}$. In this last case the difficulty is that the eigenvectors of M are not well-defined, hence the arguments where we use that the eigenvectors of \tilde{Z} converge to the eigenvectors of M do not work automatically. This can be overcome by choosing a sequence of Q 's along which the eigenvectors of \tilde{Z} do converge, and denoting their limits (which will of course still be pairwise orthogonal eigenvectors of M) by ψ_1, ψ_2, ψ_3 . Now by the arguments of Lemma 3 we still get that ψ_3 has to be parallel to $(0, 1, -1)$. Also we know that ψ_1 is parallel to $(1, 1, 1)$ since this is a 1-dimensional eigenspace of M . And then ψ_2 is parallel to $(-2, 1, 1)$. Now the corresponding eigenvalues are 2, $-1, -1$ and the arguments of Lemma 4 go through word by word. As $\gamma = 1$ in our case, and 1 is not odd-over-even, we get that the tunneling time has to satisfy $Q^a = O(f(Q))$ as before. This completes the proof of part c).

Remark 4. Now we see that by Lemma 5 the only way Conjecture 1 could be false is if there existed a graph with three of its vertices x, y, z forming an equilateral triangle such that $c_{xy} = c_{xz} \neq c_{yz}$ and $\sqrt{c_{yz}^2 + 8c_{xz}^2}$ is rational, and at the same time the ratio $(\lambda_1(Q) - \lambda_3(Q)) / (\lambda_1(Q) - \lambda_2(Q))$ is independent of Q . Though currently we are unable to prove it, we believe such graphs do not exist.

3.4. Instability.

Lemma 6. *If there is an order three symmetry of the graph that permutes the wells (in particular $c_{xy} = c_{xz} = c_{yz}$) then there is no perfect tunneling from y to z , in fact $TC(y, z) = 4/9$.*

Proof. Using the order three symmetry of the graph it is easy to see that $\tilde{Z}_{xx} = \tilde{Z}_{yy} = \tilde{Z}_{zz}$ and $\tilde{Z}_{xy} = \tilde{Z}_{yz} = \tilde{Z}_{zx}$. Hence $(1, 1, 1)$ is an eigenvector of \tilde{Z} , and the whole

subspace orthogonal to $(1, 1, 1)$ is a 2-dimensional eigenspace. This way in the decomposition of $(1, 0, 0)$ there will only be two terms: $1/3(1, 1, 1) + 1/3(2, -1, -1)$. As before, these two eigenvectors are rotating at different speeds, so after a certain amount of time (not hard to see that the order of magnitude is Q^{a-1}) their phases will be opposite, and the state of the particle becomes $1/3(-1, 2, 2)$, which will be the extremally tunneled state. Hence $TC(y, z) = 4/9$. It is also obvious that at any moment during the whole evolution the states y and z will be equally likely. \square

Proof (Proof of Theorem 4). Let us consider the following simple construction. Let our graph consist of three paths joined at a common vertex O . (So O has degree 3, the endpoints of the paths have degree 1 and all the other vertices have degree 2.) Let the three wells be the three neighbors of O . Let the length of the paths going through x, y, z be denoted respectively by a, b, c . If $a = b = c$ then by the previous lemma we get that for any two wells the tunneling coefficient is $4/9$.

On the other hand if $a \neq b = c$ then there is perfect tunneling from y to z . To see this, first we have to understand the eigenvectors of \tilde{Z} . Let us assume $a < b$, though the $a > b$ case would work just as well. It is easy to see that $\tilde{Z}_{xy} = \tilde{Z}_{xz} = \tilde{Z}_{yz}$ and by symmetry $\tilde{Z}_{yy} = \tilde{Z}_{zz}$. Since up to length $2a - 1$ the closed paths from all three wells are identical, but the paths of length $2a$ are not, $0 \neq \tilde{Z}_{xx} - \tilde{Z}_{yy} = 1/\lambda^{2a}$. Thus \tilde{Z} is of the form

$$\tilde{Z} = \begin{pmatrix} p & q & q \\ q & r & q \\ q & q & r \end{pmatrix}, \quad (49)$$

where $p \neq r$. Easy computation shows that the eigenfunctions of this matrix are $(c_1, 1, 1); (c_2, 1, 1); (0, 1, -1)$ and $c_1 \neq 0 \neq c_2$. It is also not hard to compute that all three eigenvalues are distinct. Thus, even though the eigenvalues of the corresponding M matrix are $1, -1, -1$, the system is still well-behaved, but $\gamma = 1$. Thus, by Lemma 5 in order to be able to apply Lemma 4 and conclude that there is indeed perfect tunneling from y to z , we have to check that $(\lambda_1 - \lambda_3)/(\lambda_1 - \lambda_2)$ is not a constant function of Q . If it were constant, it would be equal to its limit as $Q \rightarrow \infty$, which is precisely γ . But since $\gamma = 1$, this meant that $\lambda_2 = \lambda_3$ for all Q , which means that the inverse functions are also equal, and hence for the eigenvalues of \tilde{Z} we get that $\nu_2(\lambda) = \nu_3(\lambda)$. But this contradicts our previous observations. Hence there is perfect tunneling from y to z . \square

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