TUNNELLING AND THE PATH DECOMPOSITION EXPANSION

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ABSTRACT

We will review the use of the Path Decomposition Expansion for solving tunnelling problems, with an emphasis on those that cannot be easily dealt with by conventional techniques. New will be a rigorous proof based on Green's function techniques and the application to the groundstate energy splitting for one-dimensional supersymmetric quantum mechanics, resolving an apparent discrepancy.

1. Introduction

These lecture notes will present the Path Decomposition Expansion (PDX) and in particular its application to quantum tunnelling problems. The general idea is quite simple. One partitions the configuration space in various regions on which an appropriate Green's function is defined, each of which can be evaluated using a suitable approximation. The power of this method is of course that these approximations in general will differ for the different regions. The most obvious such a split is of course between the classically allowed and forbidden regions, as is well known from the WKB analysis. The general and multi-dimensional formalism I will describe was developed by A. Auerbach and S. Kivelson[1]. In a sense it can be seen as the multi-dimensional formulation of connection formula, which play such an essential role in the one-dimensional WKB analysis. Thus, certain aspects of the PDX had already appeared in the context of a careful one-dimensional WKB analysis[2a].

Frequently a lot of emphasis is put on the analysis around the turning points. We will show, however, that this is by no means necessary and that it is actually more suitable to "match the wavefunctions" in the classically forbidden region, not too far from the classical turning point, but nevertheless with a certain amount of arbitrariness. This yields a suitable consistency check, as the ultimate result should of course be independent of the "matching points". In itself this idea is not new[3], the usefulness of the PDX lies in it being able to deal with problems that would

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otherwise be much more difficult to deal with, as I hope to be able to demonstrate by explicit examples.

In section 2 we will first give a new and *rigorous* proof of the PDX using Green's function techniques. This proof is in essence based on a result from ref. 4. Then we give the path integral derivation, which will explain the origin of the method's name. In section 3 we describe how the PDX can be applied to the problem of tunnelling between degenerate minima. For purposes of clarity we will be quite detailed about some essential aspects of the derivation and illustrate its use for a few one-dimensional examples. In section 4 we first carefully evaluate the relevant integrals in the multi-dimensional case, using steepest descent methods. The explicit examples[5] we will discuss do not allow a particular adiabatic approximation, that would have allowed us to reduce the problem to one dimension. The first example involves a two-dimensional situation without a classical barrier separating the regions where in lowest order in the coupling constant ($\hbar$) the wavefunction will be localized. It involves tunnelling through a quantum induced potential barrier. The second example involves a three-dimensional potential with conic, hence not quadratic, minima. Also we discuss a new two-dimensional example, in which the failure of the adiabatic approximation is not as dramatic as in the previous two examples. Applying the adiabatic approximation in this example yields a finite, often quite small, relative error (i.e. the error does not vanish as $\hbar$ tends to zero).

In section 5 we go back to one dimension and consider the special case of supersymmetric quantum mechanics, which can be reformulated as an ordinary quantum mechanics problem. The particular interest in this problem arises due to the fact that for the groundstate energy splitting, the naive application of the WKB analysis, will give a result that differs from the supersymmetric analysis involving steepest descent techniques for path integrals containing Grassman variables[6]. As non of the students has handed in this homework assignment, we will show how the PDX can be used to correctly compute the energy split.

2. Derivation of the Path Decomposition Expansion

Let us consider a situation where configuration space is divided in two regions, inside and outside the surface Σ, as in figure 1. To allow for the presence of an electromagnetic field we will take the Hamiltonian of the form

$$H = \frac{1}{2m}(\frac{\hbar}{i}\frac{\partial}{\partial \mathbf{x}} - \frac{e}{c}\mathbf{A}(\mathbf{x}))^2 + V(\mathbf{x}). \tag{1}$$

The (energy) Green's function $G(\mathbf{x}_f, \mathbf{x}_i; E)$ is defined through the equations

$$(H(\mathbf{x}) - E)G(\mathbf{x}, \mathbf{y}; E) = (H(\mathbf{y})^* - E)G(\mathbf{x}, \mathbf{y}; E) = \hbar\delta(\mathbf{x} - \mathbf{y}). \tag{2}$$

In operator form the Green's function is given by

$$G(E) = \frac{1}{H - E - i\varepsilon}. \tag{3}$$

Now, following Inglesfield[4], let $G^{(r)}$ be any Green's function outside of the surface Σ (we will specify the boundary conditions latter, presently they can be arbitrary). There are two situations of interest. First take $\mathbf{x}$ and $\mathbf{y}$ outside of Σ and use the trivial identity

$$\begin{aligned} G^{(r)}(\mathbf{y},\mathbf{z};E)\{(H(\mathbf{z})-E)G(\mathbf{z},\mathbf{x};E)-\hbar\delta(\mathbf{z}-\mathbf{x})\} &= \\ \{(H(\mathbf{z})^{*}-E)G^{(r)}(\mathbf{y},\mathbf{z};E)-\hbar\delta(\mathbf{y}-\mathbf{z})\}G(\mathbf{z},\mathbf{x};E). & \qquad (4) \end{aligned}$$

Integrating over $\mathbf{z}$ in the region outside of Σ is easily seen to result in the following equation

$$G(\mathbf{y},\mathbf{x};E)=G^{(r)}(\mathbf{y},\mathbf{x};E)+\int_{\Sigma}d_{\Sigma}\mathbf{z}\ G^{(r)}(\mathbf{y},\mathbf{z};E)[\Sigma(\mathbf{z})]G(\mathbf{z},\mathbf{x};E), \qquad (5)$$

where we have introduced for later convenience the (hermitian) surface operator

$$[\Sigma(\mathbf{z})]=\frac{i}{2}\mathbf{n}(\mathbf{z})\cdot(\overrightarrow{\mathbf{p}(\mathbf{z})}-\overleftarrow{\mathbf{p}(\mathbf{z})}^{*}), \quad \mathbf{p}(\mathbf{z})=(\frac{\hbar}{i}\frac{\partial}{\partial\mathbf{z}}-\frac{e}{c}\mathbf{A}(\mathbf{z}))/m, \qquad (6)$$

with $\mathbf{n}(\mathbf{z})$ the outward normal on the surface Σ. It is not surprising that the covariant momentum operator appears, since gauge invariance has to be maintained. On the other hand if we take $\mathbf{x}$ inside and $\mathbf{y}$ outside of Σ the same identity as in eq.(4) holds, except that now $G^{(r)}(\mathbf{y},\mathbf{x};E)$ will always vanish, such that

$$G(\mathbf{y},\mathbf{x};E)=\int_{\Sigma}d_{\Sigma}\mathbf{z} \quad G^{(r)}(\mathbf{y},\mathbf{z};E)[\Sigma(\mathbf{z})]G(\mathbf{z},\mathbf{x};E). \qquad (7)$$

Restricting to the case of vanishing boundary conditions for $G^{(r)}(\mathbf{y},\mathbf{x};E)$ provides a rigorous derivation of the PDX, even in the presence of a vector potential (which from now on will be ignored again), using Green's function techniques. Here

Figure 1: Sketch of the PDX for eq. (7), where $\mathbf{x}_i = \mathbf{x}$ is inside and $\mathbf{x}_f = \mathbf{y}$ outside of Σ, with $\mathbf{x}_\sigma = \mathbf{z}$ on the surface of Σ. The solid path from $\mathbf{x}_i$ to $\mathbf{x}_\sigma$ contributes to $G(\mathbf{z},\mathbf{x};E)$, whereas the dashed path, which is restricted never to cross the surface of Σ, contributes to $G^{(tr)}(\mathbf{y},\mathbf{z};E)$. (This is fig. 1.1.a from ref. [1a]).

we have considered the case where configuration space is split in two regions. Typically this will be applicable to a potential with a single minimum, where we choose the surface Σ such that the classically allowed region is fully contained inside this surface. This means that $G^{(r)}$ can be computed with standard steepest descent techniques, whereas $G(\mathbf{z},\mathbf{x};E)$ can be evaluated with standard perturbative techniques. The latter guarantee convergence in the L^2 sense and because $\mathbf{z}$ will not become too large, this usually means control over the relative error at $\mathbf{z}$. It is also clear that the Green's function technique can be generalized to arbitrary divisions of configuration space, a generalization that will be used for the tunnelling problem.

We now come to the path integral derivation[1] of the PDX, which is intuitively more appealing, but less rigorous. In path integrals the evolution operator $\exp(-iHt)$, or its kernel $K(\mathbf{y},\mathbf{x};t)$, is the more natural object to consider. We will assume the reader is familiar with path integrals[7,8]. The evolution Kernel satisfies the Schrödinger equation $(H-i\hbar\partial_t)K(\mathbf{y},\mathbf{x};t)=0$ with the boundary condition $\lim_{t\to 0}K(\mathbf{y},\mathbf{x};t)=\delta(\mathbf{x}-\mathbf{y})$ and the energy Green's function is related to this kernel by the "Laplace transform"

$$G(\mathbf{y},\mathbf{x};E)=i\int_0^\infty dt\ K(\mathbf{y},\mathbf{x};t)e^{iE(t+i\varepsilon)/\hbar}. \tag{8}$$

This allows us to rewrite the Green's function identities in terms of the evolution kernels. For example if $\mathbf{x}$ is inside and $\mathbf{y}$ outside of Σ one easily finds

$$K(\mathbf{y},\mathbf{x};T)=i\int_0^T dt\int_\Sigma d_\Sigma\mathbf{z}\quad K^{(r)}(\mathbf{y},\mathbf{z};t)[\Sigma]K(\mathbf{z},\mathbf{x};T-t). \tag{9}$$

To interpret this PDX formula in terms of path integrals, we note that the evolution kernel equals the Feynman-Kac sum over paths $\mathbf{x}(t)$, weighed with $\exp[iS(\mathbf{x}(t))/\hbar]$, where $S(\mathbf{x}(t))=\int_0^T dt\{\frac{1}{2}m\dot{\mathbf{x}}(t)^2-V(\mathbf{x}(t))\}$ is the classical action, or

$$K(\mathbf{y},\mathbf{x};T)=\int_{\mathbf{x}(0)=\mathbf{x}}^{\mathbf{x}(T)=\mathbf{y}}\mathcal{D}\mathbf{x}(t)\exp[iS(\mathbf{x}(t))/\hbar]. \tag{10}$$

By definition $K^{(r)}$ is defined in terms of $G^{(r)}$ as in eq. (8). It will therefore vanish at the surface Σ and the path integral expression for $K^{(r)}$ will involve integration over those paths that will never cross the surface Σ, thereby explaining the label (r), meaning restricted.

Hence eq. (9) can be phrased by saying that the probability for propagating from $\mathbf{x}$ to $\mathbf{y}$ is decomposed as the probability to first propagate in a time t to a point $\mathbf{z}$ on Σ and from thereon propagate to $\mathbf{y}$ in the remaining time *without ever crossing* Σ *again*. The time t is for each classical path the moment of last crossing of Σ and thereby unambiguous. As t and $\mathbf{z}$ are arbitrary we have to integrate over them. One can argue that the operator $[\Sigma]$ has to appear to make integration over Σ well defined. More convincingly, $[\Sigma]$ is exactly the operator for the current across the surface Σ and its presence is to insure "conservation of probability across the surface". For an alternative justification see ref. 1. The interpretation in terms of probability can be even made more precise by performing the famous Wick rotation to imaginary time $t \to -it$, where the path integral can be rigorously defined in terms of the Wiener measure. The relevant kernel $K(\mathbf{y},\mathbf{x},-it)$ is appropriately called the heat kernel. In terms of the euclidean action $S_{eucl}(\mathbf{x}(t)) = \int_0^T dt\{\frac{1}{2}m\dot{\mathbf{x}}(t)^2 + V(\mathbf{x}(t))\}$ it is given by

$$K_{eucl}(\mathbf{y},\mathbf{x},T) \equiv K(\mathbf{y},\mathbf{x};-iT) = \int_{\mathbf{x}(0)=\mathbf{x}}^{\mathbf{x}(T)=\mathbf{y}} \mathcal{D}\mathbf{x}(t)\exp[-S_{eucl}(\mathbf{x}(t))/\hbar]. \tag{11}$$

and satisfies, e.g. for $\mathbf{x}$ inside and $\mathbf{y}$ outside of Σ, the following equivalent of eq. (9)

$$K_{eucl}(\mathbf{y},\mathbf{x};T) = -\int_0^T dt \int_\Sigma d_\Sigma \mathbf{z}\; K^{(r)}_{eucl}(\mathbf{y},\mathbf{z};t)[\Sigma]K_{eucl}(\mathbf{z},\mathbf{x};T-t). \tag{12}$$

It is this version of the PDX that we will derive using the path integral. We will first discuss the one-dimensional case, where the discretized version of K_{eucl} is given by

$$\begin{aligned}
K_N(y,x,T) &= (\frac{m}{2\pi\hbar\varepsilon})^{N/2}\int_{-\infty}^{\infty}\prod_{i=1}^{N-1}dx_i\;\exp\Bigl(-\frac{1}{\hbar}\sum_{j=0}^{N-1}U_\varepsilon(x_j,x_{j+1})\Bigr),\\
U_\varepsilon(x_j,x_{j+1}) &= \frac{m}{2\varepsilon}(x_{j+1}-x_j)^2+\varepsilon V(x_j),
\end{aligned} \tag{13}$$

with $x_0 = x$, $x_N = y$ and $T = \varepsilon N$. Here we have divided the time interval T in N equal pieces, but an essential aspect of proving the existence of the Wiener integral is to show that $K_{eucl} = \lim_{N\to\infty} K_N$ is independent of the partitioning of this interval. For deriving the PDX this will turn out not to be an academic remark.

The last moment of crossing $\Sigma \equiv \{z\}$ can occur in any of the time intervals $[i\varepsilon,(i+1)\varepsilon]$, which leads to the trivial identity

$$\begin{aligned}
K_N(y,x,T) = &\sum_{i=0}^{N-1}(\frac{m}{2\pi\hbar\varepsilon})^{N/2}\int_{-\infty}^{\infty}\prod_{j=1}^{i-1}dx_j\;\exp\Bigl(-\frac{1}{\hbar}\sum_{j=0}^{i-1}U_\varepsilon(x_j,x_{j+1})\Bigr)\times\\
&\int_{-\infty}^{z}dx_i\;\exp\Bigl(-\frac{1}{\hbar}U_\varepsilon(x_i,x_{i+1})\Bigr)\int_z^{\infty}\prod_{j=i+1}^{N-1}dx_j\;\exp\Bigl(-\frac{1}{\hbar}\sum_{j=i+1}^{N-1}U_\varepsilon(x_j,x_{j+1})\Bigr).
\end{aligned} \tag{14}$$

The following identity will be very useful[1]

$$\begin{aligned}
\sqrt{\frac{m}{2\pi\hbar\varepsilon}}\exp\Bigl(-\frac{m(x_{i+1}-x_i)^2}{2\hbar\varepsilon}\Bigr) = &\int_0^\varepsilon d\tau\sqrt{\frac{m}{2\pi\hbar\tau}}\exp\Bigl(-\frac{m(z-x_i)^2}{2\hbar\tau}\Bigr)\times\\
&\frac{\hbar}{m}\frac{\partial}{\partial z}\Bigl\{\sqrt{\frac{m}{2\pi\hbar(\varepsilon-\tau)}}\exp\Bigl(-\frac{m(x_{i+1}-z)^2}{2\hbar(\varepsilon-\tau)}\Bigr)\Bigr\},
\end{aligned} \tag{15}$$

as it allows us to write

$$K_N(y,x,T) = \sum_{i=0}^{N-1} \int_0^\varepsilon d\tau \ (\frac{m}{2\pi\hbar\varepsilon})^{i/2} \sqrt{\frac{m}{2\pi\hbar\tau}} \int_{-\infty}^{\infty} \prod_{j=1}^{i-1} dx_j \int_{-\infty}^{z} dx_i \ \times$$
$$\exp\Bigl(-\frac{1}{\hbar}[U_\tau(x_i,z) + \sum_{j=0}^{i-1} U_\varepsilon(x_j,x_{j+1})\Bigr) \frac{\hbar}{m}\frac{\partial}{\partial z}\{R(\frac{m}{2\pi\hbar\varepsilon})^{(N-i-1)/2}\sqrt{\frac{m}{2\pi\hbar(\varepsilon-\tau)}}\times$$
$$\int_z^\infty \prod_{j=i+1}^{N-1} dx_j \ \exp\Bigl(-\frac{1}{\hbar}[U_{\varepsilon-\tau}(z,x_{i+1}) + \sum_{j=i+1}^{N-1} U_\varepsilon(x_j,x_{j+1})]\Bigr)\}, \tag{16}$$

where $R = \exp\{-(\varepsilon-\tau)[V(x_i) - V(z)]/\hbar\}$. In path integrals coordinate differences behave as $\sqrt{\varepsilon}$, such that in the continuum limit R will not contribute, so we will put $R = 1$. Similarly

$$\int_z^\infty dx_i \ \exp(-U_\tau(x_i,z)/\hbar) = \int_{-\infty}^z dx_i \ \exp(-U_\tau(x_i,z)/\hbar)\hat{R},$$

with $\hat{R} = \exp\{-\tau[V(2z - x_i) - V(x_i)]/\hbar\}$, which can also be put to one in the continuum limit. Thus, $\int_z^\infty dx_i$ can be replaced by $\frac{1}{2}\int_{-\infty}^\infty dx_i$ and we find

$$K_N(y,x;T) = \int_0^T dt \ K_{N_1}(z,x;t)\frac{\hbar}{2m}\frac{\partial}{\partial z}K_{N_2}^{(r)}(y,z;T-t), \tag{17}$$

where K_{N_1} corresponds to the partitioning of t in i intervals of length ε and a last interval of length $\tau < \varepsilon$, whereas $K_{N_2}^{(r)}$ corresponds to the partioning of $T - t$ in $N - i - 1$ intervals of length ε and a first interval of length $\varepsilon - \tau$ *and* a restriction of configuration space to $x \geq z$. Thus, as the Wiener integrals are independent of the chosen partitionings, one obtains the required result of eq. (12) in the continuum limit $N \to \infty$.

To complete the path integral derivation we first need to prove eq. (15). The Laplace transform with respect to t of

$$f(x;t) = \sqrt{\frac{m}{2\pi\hbar t}}\exp(-\frac{mx^2}{\hbar t}) \tag{18}$$

is given by

$$\hat{f}(x;\lambda) = \int_0^\infty dt \ f(x;t)e^{-\lambda t} = \sqrt{\frac{m}{2\hbar\lambda}}\exp\Bigl(-|x|\sqrt{2m\lambda/\hbar}\Bigr). \tag{19}$$

Hence we find for the Laplace transform of the rhs. of eq.(15) ($t \equiv \varepsilon$),

$$\int_0^\infty dt \ e^{-\lambda t}\int_0^t d\tau \ f(z - x_i;\tau)\frac{\hbar}{m}\frac{\partial}{\partial z}f(x_{i+1} - z; t-\tau). \tag{20}$$

Using the convolution theorem and eq. (19), this becomes

$$\hat{f}(z-x_i;\lambda)\frac{\hbar}{m}\frac{\partial}{\partial z}\hat{f}(x_{i+1}-z;\lambda)=\sqrt{\frac{m}{2\hbar\lambda}}\exp\Bigl(-|x_{i+1}-x_i|\sqrt{2m\lambda/\hbar}\Bigr), \tag{21}$$

which is exactly the Laplace tranform of the lhs. of eq. (15). Finally, to generalize the proof to higher dimensions, we decompose at the surface Σ the coordinates in a component perpendicular to the surface and components tangent to the surface. For each of the latter components we use another remarkable identity[1]

$$\begin{aligned}\sqrt{\frac{m}{2\pi\hbar\varepsilon}}\exp\Bigl(-\frac{m(x-y)^2}{2\hbar\varepsilon}\Bigr)=\int_{-\infty}^{\infty}dz\sqrt{\frac{m}{2\pi\hbar\tau}}\exp\Bigl(-\frac{m(z-x)^2}{2\hbar\tau}\Bigr)\times\\ \sqrt{\frac{m}{2\pi\hbar(\varepsilon-\tau)}}\exp\Bigl(-\frac{m(z-x)^2}{2\hbar(\varepsilon-\tau)}\Bigr),\end{aligned} \tag{22}$$

which follows directly from the Gaussian integration over z.

It should be clear that, despite the ingeneous indentities of eqs. (15) and (22), a much harder analysis is required to make the path integral derivation mathematically justifiable. We will leave this as a challenge to the path integral aficionado, ourselves being satisfied with the *rigorous* proof based on the elegant Green's function technique.

To prepare the ground for the next section, we end this one by using the PDX to give an amusingly simple proof[9] of the method of images to construct $G^{(r)}$ such that it vanishes at the boundary Σ. Note that the restriction of the paths in the path integral expression of $K^{(r)}$ can be imposed by taking the potential infinite inside Σ. Similarly, such a change in the potential will force vanishing boundary conditions for $G^{(r)}$ at Σ, when solving the Schrödinger equation. For convenience we take for Σ a plane defined by $x_1=0$. If P represents reflection in Σ, we define $V^{(u)}(\mathbf{x})=V(\mathbf{x})$ for $x_1\geq 0$ and $V^{(u)}(\mathbf{x})=V(P\mathbf{x})$ for $x_1\leq 0$. Its Green's function $G^{(u)}$ satisfies

$$G^{(u)}(\mathbf{z},\mathbf{x};E)=G^{(u)}(\mathbf{z},P\mathbf{x};E),\quad \text{for}\quad z_1=0 \tag{23}$$

The PDX gives for $x_1\geq 0$ and $y_1\geq 0$

$$\begin{aligned}G^{(u)}(\mathbf{y},\mathbf{x};E)&=-\int_\Sigma d_\Sigma\mathbf{z}\;G^{(u)}(\mathbf{z},\mathbf{x};E)\frac{\hbar}{2m}\frac{\partial}{\partial z_1}G^{(r)}(\mathbf{y},\mathbf{z};E)+G^{(r)}(\mathbf{y},\mathbf{x};E)\\ G^{(u)}(\mathbf{y},P\mathbf{x};E)&=-\int_\Sigma d_\Sigma\mathbf{z}\;G^{(u)}(\mathbf{z},P\mathbf{x};E)\frac{\hbar}{2m}\frac{\partial}{\partial z_1}G^{(r)}(\mathbf{y},\mathbf{z};E),\end{aligned} \tag{24}$$

The required result

$$G^{(r)}(\mathbf{y},\mathbf{x};E)=G^{(u)}(\mathbf{y},\mathbf{x};E)-G^{(u)}(\mathbf{y},P\mathbf{x};E). \tag{25}$$

is obtained by subtracting these two equations and using eq. (23).

3. Application to the problem of tunnelling

We will now consider the situation where the potential has two degenerate minima, in which case it is most natural to divide space in three different regions separated by two different surfaces Σ_1 and Σ_2, where the classically allowed regions are enclosed by these two surfaces, see figure 2. The enclosed regions that contain a minimum of the potential will be called well regions or wells, for short. We can now distinguish three different types of restricted Green's functions, $G^{(1)}$ and $G^{(2)}$ with vanishing boundary conditions on Σ_2, resp. Σ_1, and $G^{(tr)}$ with vanishing boundary conditions at both surfaces. The latter describes the paths that make the transition through the classically forbidden region from one well to the other. The transition Green's function $G^{(tr)}$ will therefore be approximated by a steepest descent calculation, see further on. As we have seen in the derivation of the PDX through the Green's function technique, we are not forced to take vanishing boundary conditions on the various Green's function. It will turn out that we shall never use the behaviour of $G^{(i)}$ near the boundary of its domain, but for $G^{(tr)}$ it is useful to remember that we have other options. To keep the notations as efficient as possible we will use the operator form, eq. (3), of the Green's function and likewise write (compare eq. (6)),

$$[\Sigma] = \int_\Sigma d_\Sigma \mathbf{z}\ |z > [\Sigma(\mathbf{z})] < z|. \tag{26}$$

Let us analyse in detail the case where $\mathbf{x}$ is in well 1 and $\mathbf{y}$ in well 2. Hopefully the reader will not decompose before we have reached the end of eq. (27); please bear with me on this one, it'll be worthwhile. First apply eq. (7) for $\{G,\ G^{(2)}\}$ to

Figure 2: Sketch of the PDX for the tunnelling case. The dashed-dotted-dashed line indicates a typical contribution to the bounce $G_b^{(2)}$ of eq. (29), composed of the dashed lines that contribute to $G^{(tr)}$ in resp. M and $M^\dagger$ (eq. (28)) and the dotted line that contributes to $G^{(2)}$. The solid line gives the dominating contribution to M, and plays a role in the explicit evaluation of the tunnelling amplitude in section 4 ($\bar{\mathbf{x}}(t) = \mathbf{x}_0(t)$, $\bar{\mathbf{x}}_{\sigma_1} = \mathbf{x}_0$ and $\bar{\mathbf{x}}_{\sigma_2} = \mathbf{y}_0$). (This is fig. 1.4 from ref. [1a]).

find (the explicit E dependence will usually be suppressed)

$$< \mathbf{y}|G|\mathbf{x} >=< \mathbf{y}|G^{(2)}[\Sigma_1]G|\mathbf{x} >, \tag{27a}$$

next apply eq. (5) for $\{G,\ G^{(1)}\}$,

$$< \mathbf{y}|G|\mathbf{x} >=< \mathbf{y}|G^{(2)}[\Sigma_1]G^{(1)} + G^{(2)}[\Sigma_1]G^{(1)}[\Sigma_2]G|\mathbf{x} >, \tag{27b}$$

then apply the *conjugate* of eq. (7) for $\{G^{(1)},\ G^{(tr)}\}$ and define

$$M(E) = [\Sigma_1]G^{(tr)}(E)[\Sigma_2], \quad M(E)^\dagger = [\Sigma_2]G^{(tr)}(E)[\Sigma_1], \tag{28}$$

to obtain

$$< \mathbf{y}|G|\mathbf{x} >=< \mathbf{y}|G^{(2)}[\Sigma_1]G^{(1)} + G^{(2)}[\Sigma_1]G^{(1)}MG|\mathbf{y} > . \tag{27c}$$

Following this use again eq. (7) for $\{G,\ G^{(2)}\}$ to find

$$< \mathbf{y}|G|\mathbf{x} >=< \mathbf{y}|G^{(2)}[\Sigma_1]G^{(1)} + G^{(2)}[\Sigma_1]G^{(1)}MG^{(2)}[\Sigma_1]G|\mathbf{x} >, \tag{27d}$$

and finally application of the *conjugate* of eq. (7) for $\{G^{(2)},\ G^{(tr)}\}$ yields

$$< \mathbf{y}|G|\mathbf{x} >=< \mathbf{y}|G^{(2)}[\Sigma_1]G^{(1)} + G^{(2)}[\Sigma_1]G^{(1)}G_b^{(2)}G|\mathbf{x} >, \tag{27e}$$

where we have introduced the so-called bounce operator

$$G_b^{(2)}(E) = M(E)G^{(2)}(E)M(E)^\dagger, \quad G_b^{(1)}(E) = M(E)^\dagger G^{(1)}(E)M(E). \tag{29}$$

By repeating the steps (27b) through (27e), we can iterate this result and together with (apply the *conjugate* of eq. (7) for $\{G^{(2)}, G^{(tr)}\}$, remember that $\mathbf{y}$ is in well 2)

$$< \mathbf{y}|G^{(2)}[\Sigma_1]G^{(1)} =< \mathbf{y}|G^{(2)}M^\dagger G^{(1)}, \tag{30}$$

one finds

$$< \mathbf{y}|G|\mathbf{x} >=< \mathbf{y}|G^{(2)}M^\dagger G^{(1)}(1 - G_b^{(2)}G^{(1)})^{-1}|\mathbf{x} > . \tag{27f}$$

This expresses the Green's function as the sum over all possible transitions $M(E)$ from one well to the other well. These transitions occur in pairs (the bounce $G_b^{(i)}$) and the propagation in well i is described by $G^{(i)}$, which - and that is essential - we only need to know accurately within the wells (whereas they are defined over the whole region excluding the other well. It forms the rational behind the use of eq. (30).)

After having discussed the interpretation of the PDX we can consider the other cases without too much difficulty. First, however, observe that we could have started with $< \mathbf{y}|G|\mathbf{x} >=< \mathbf{y}|G[\Sigma_2]G^{(1)}|\mathbf{x} >$, rather than eq. (27a), which after iteration would yield (simply interchange the labels 1 and 2 and the two coordinates in the complex conjugate of eq. (27f))

$$< \mathbf{y}|G|\mathbf{x} >=< \mathbf{y}|(1 - G^{(2)}G_b^{(1)})^{-1}G^{(2)}M^\dagger G^{(1)}|\mathbf{x} > . \tag{27g}$$

It is easily seen that this indeed coincides with eq. (27f). Now consider the case where $\mathbf{x}$ and $\mathbf{y}$ are both in well 1. This gives the following expansion

$$< \mathbf{y}|G|\mathbf{x} >=< \mathbf{y}|(1 - G^{(1)}G_b^{(2)})^{-1}G^{(1)}|\mathbf{x} > . \tag{31}$$

The case were $\mathbf{x}$ is in well 2 and $\mathbf{y}$ in well 1 is obtained from eq. (27f) by interchanging the two labels and the case where both $\mathbf{x}$ and $\mathbf{y}$ are in well 2 can similarly be obtained from eq. (31). If we now introduce the notation $\mathbf{x}^{(i)}$ if $\mathbf{x}$ is in well i, we can define the direct sum of the two spaces, spanned by $\{|\mathbf{x}^{(1)} > \oplus|\mathbf{x}^{(2)} >\}$. With respect to that basis the four cases we have computed above can be conveniently captured by (note that $H(\mathbf{x}^{(i)}) - E - i\varepsilon = \hbar G^{(i)}(E)^{-1}$)

$$< \mathbf{y}^{(i)}|G(E)|\mathbf{x}^{(j)} >= \hbar < \mathbf{y}^{(i)}|(\mathcal{H}(E) - E - i\varepsilon)^{-1}|\mathbf{x}^{(j)} >, \tag{32}$$

where the energy dependent hermitian "Hamiltonian" $\mathcal{H}(E)$ is given by.

$$\mathcal{H}(E) = \begin{pmatrix} H & -\hbar M(E) \\ -\hbar M(E)^\dagger & H \end{pmatrix} \tag{33}$$

The proof is almost trivial, and the result is intuitively very appealing as it makes precise that the perturbation due to the transitions between the wells is given by the overlap of the wavefunctions in the barrier region, as will become more obvious further on.

We should point out that eq. (32) is no longer valid if either of the coordinates is taken in the transition region, i.e. in neither of the wells (as was inadvertently claimed in ref. 1). This is obvious, for in the case that both points are in neither well, the leading decomposition of the Green's function should include $G^{(tr)}(E)$. To be more precise we can consider $\mathbf{x}^{(i)}$ to cover the domain of definition of $G^{(i)}$, e.g. $\mathbf{x}^{(1)}$ describes the region outside of well 2. Whenever we used eq. (7) for the manipulations involving eq. (27), we often will have to use eq. (5) instead. Careful but straightforward bookkeeping will yield the following result - a result that also follows by simply summing over all possible transitions -

$$\begin{aligned} < \mathbf{y}^{(2)}|G|\mathbf{x}^{(1)} > =< \mathbf{y}^{(2)}|[1 + G^{(tr)}[\Sigma_1]G^{(1)}M]G^{(2)}\{1 - G_b^{(1)}G^{(2)}\}^{-1}[\Sigma_2]G^{(tr)} \\ + [G^{(tr)}[\Sigma_1] + G^{(2)}M^\dagger]G^{(1)}\{1 - G_b^{(2)}G^{(1)}\}^{-1} + G^{(r)}|\mathbf{x}^{(1)} > \end{aligned} \tag{34}$$

Remarkably, it is still possible to find a simple expression like eq. (32). It should be noticed that the the basis $\{|\mathbf{x}^{(1)} > \oplus|\mathbf{x}^{(2)} >\}$ is now overcomplete, but this does not really harm us (it would be more harmful not to cover the transition region $\cdots$). The full result is found to be

$$< \mathbf{y}^{(j)}|G(E)|\mathbf{x}^{(i)} >= \hbar < \mathbf{y}^{(j)}|G^{(tr)}(E) + B(E)^\dagger(\mathcal{H}(E) - E - i\varepsilon)^{-1}B(E)|\mathbf{x}^{(i)} >, \tag{35}$$

with a matrix $B(E)$ of the following simple form

$$B(E) = \begin{pmatrix} 1 & [\Sigma_1]G^{(tr)}(E) \\ [\Sigma_2]G^{(tr)}(E) & 1 \end{pmatrix} \tag{36}$$

Now comes the crucial remark[1] that the energy eigenvalues of the full problem are found as the poles of $G(E)$. Since poles in $G^{(tr)}(E)$ are spurious, the physical spectrum comes from the energy dependent Hamiltonian $\mathcal{H}(E)$ and we see that the omission of $B(E)$ has no consequences for the spectrum (but it does affect the wavefunctions).

As the off-diagonal elements are expected to be exponentially small for a typical tunnelling problem, one can do first order perturbation theory. For $|\Psi_n^{(i)} >\equiv |n^{(i)}>$ and $E_n^{(i)}$, respectively the eigenfunctions and eigenvalues for the two wells, i.e.

$$G^{(i)}(E) = \hbar \sum_n \frac{|\Psi_n^{(i)} >< \Psi_n^{(i)}|}{E_n^{(i)} - E - i\varepsilon}, \tag{37}$$

the off-diagonal matrix elements are expressed in terms of $< n^{(1)}| - \hbar M(E)|n^{(2)} >$. The simplest case arises for a symmetric potential that has an exact degeneracy when transitions are neglected if we choose the decomposition surfaces Σ_i to be arranged symmetrically. The energy shift in this case is exponential and we can safely substitute $E = E_n^{(i)}$ in the matrix element of $M(E)$, such that ordinary degenerate perturbation theory yields

$$E_n = E_n^{(i)} \pm \hbar| < n^{(2)}|M(E_n^{(i)})|n^{(1)} > |. \tag{38}$$

It should be emphasized that this result is also true for excited states.

Generalization to metastable situations[2a,10] is straightforward, also the computation of the decay width (see e.g. ref. 2b and for a particularly interesting resonant situation ref. 2c) in the formalism of the PDX is in principle possible[1], but will not be pursued here. Much of the remainder of these notes will be used to show that one can now go beyond many of the limitations (like quadratic minima) of the early multi-dimensional tunnelling analysis[11] (see also references in ref. 1,2,3,5,10). For many more applications we refer the reader to ref. 1. We end this section by applying the formalism to simple one-dimensional double-well problems to warm up and to demonstrate how the freedom of choosing the decomposition surfaces (cq. points) Σ_i avoids the problems around the classical turning points. Also we show that chosing $G^{(tr)}$ with non-vanishing boundary conditions will give the same result.

So let us consider one of the simplest double-well potentials

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{8}m\omega^2(x^2-a^2)^2. \tag{39}$$

It is customary to rescale the coordiantes and the time to be dimensionless. After such a scaling this Hamiltonian is of the form

$$H = -\frac{g^2}{2}\frac{d^2}{dx^2} + \frac{1}{8}(x^2-1)^2 \tag{40}$$

and g is a dimensionless coupling constant. The rational behind this is that the tunnelling analysis yields an asymptotic expansion in $\hbar$. As $\hbar$ has a dimension, the relevant expansion parameter is only found by forming a dimensionless ratio. In this particular example one restores the dependence on the original parameters by multiplying all energies with $m\omega^2 a^4$ and substituting $g = \hbar/(m\omega a^3)$. The PDX formula relevant for eq. (40) are obtained by putting $\hbar = g$ and $m = 1$. First we compute the energy split between the even and odd states (for an arbitrary level)

$$\Delta E_n = 2g|<n|M(E_n)|n>| \tag{41}$$

using vanishing boundary conditions on $G^{(tr)}$. We choose the decomposition points $\Sigma_1 = d{-}1$ and $\Sigma_2 = 1{-}d$ and construct the transition Green's function with the method of multiple images, similarly to what was discussed at the end of the previous section. The multiple reflections are given by

$$P_k x = 2k(1-d) + (-1)^k x \tag{42}$$

and the potential $V^{(u)}$ we get by multiple reflections is thus defined by

$$V^{(u)}(P_k x) = V(x), \quad \text{for} \quad |x| \leq 1{-}d. \tag{43}$$

In terms of the associated Green's function $G^{(u)}$ one easily checks that

$$G^{(tr)}(y,x;E) = \sum_{k\in\mathbb{Z}} (-1)^k G^{(u)}(y, P_k x; E), \tag{44}$$

by verifying its vanishing at $|x| = 1{-}d$. The Green's function $G^{(u)}$ can now be evaluated with standard steepest descent methods[8], i.e. in one dimension by ordinary WKB. We find

$$\begin{aligned}\Delta E_n &= \frac{g^3}{2}|\Psi_n^{(2)}(y)^*\{\frac{d^2}{dxdy}G^{(tr)}(y,x;E_n)\}\Psi_n^{(1)}(x)|_{y=-x=1-d} \\ &= 2g^3|\Psi_n(y)|^2|\{\frac{d^2}{dxdy}G^{(u)}(y,x;E_n)\}|_{y=-x=1-d}.\end{aligned} \tag{45}$$

We have used the symmetry to put $|\Psi_n^{(1)}(x)| = |\Psi_n^{(2)}(-x)| \equiv |\Psi_n(x)|$ and the fact that in the WKB approximation of eq. (44), where $G^{(u)}(y,x;E)$ decays approximately exponential with $|x-y|$, only four terms in the sum over k are of the same order, the other terms give corrections roughly of the order of ΔE_n^2 and can be neglected. It is clear that we can immediately generalize these results to higher dimensions when we choose the decomposition surfaces Σ_i to be hypersurfaces of codimension one, perpendicular to the line connecting the two minima. The multiple reflections are now considered in the direction of this line and, apart from an integration over the surfaces, the result is identical to the one given in eq.(45) (see the next section for further details). Sometimes it might be quite awkward to have to choose Σ_i in the form of hyperplanes that extend to infinity. As emphasized before, the vanishing boundary conditions of $G^{(tr)}$ is not a fundamental property. If we replace $G^{(tr)}$ by a Green's function $G^{(e)}$, defined by smoothly extending the potential beyond the transition region, (usually such that $V \gg E$ everywhere within the wells,) eq. (45) will simply be replaced by

$$\Delta E_n = \frac{g^3}{2}|\Psi_n^{(2)}(y)^*(\overrightarrow{\frac{d}{dy}} - \overleftarrow{\frac{d}{dy}})G^{(e)}(y,x;E_n)(\overrightarrow{\frac{d}{dx}} - \overleftarrow{\frac{d}{dx}})\Psi_n^{(1)}(x)|_{y=-x=1-d} \tag{46}$$

But if we choose the surfaces Σ_i deep enough in the classically forbidden region and let the extended potential coincide in a full neighborhood of Σ_i with the original potential, then the two-sided derivative can be replaced by twice the one-sided derivative. This easily follows from the explicit WKB analysis of both quantities.

After these general remarks, equally valid for the multi-dimensional case, we return to our one-dimensional example, eq. (40). In any standard textbook on quantum mechanics one finds that

$$G^{(u)}(y,x;E) \sim [4(V(x)-E)(V(y)-E)]^{-\frac{1}{4}} \exp\Big(-\frac{1}{g}\int_x^y dz\ \sqrt{2(V(z)-E)}\Big), \tag{47}$$

which implies

$$|\{\frac{d^2}{dxdy}G^{(u)}(y,x;E)\}|_{y=-x} = \frac{1}{g^2}\sqrt{2(V(x)-E)}\exp\Big(-\frac{1}{g}|\int_{-x}^{x} dz\ \sqrt{2(V(z)-E)}|\Big). \tag{48}$$

It is not too difficult to make accurate estimates for the relative error in this asymptotic result[5], in this case it is of the order $e_{sc} \equiv g/d^2$. This makes one wish to take d as large as possible. On the other hand, if we don't make d too large, we can approximate $\Psi_n(1-d)$ by ignoring the higher order terms in the potential near the minimum. The lowest order approximation of the potential around the minimum is given by the so-called single-well potential (we shift the origin to $x=1$) $V^{[0]}(x) = x^2/2$, i.e. the simple harmonic oscillator. If we choose d such that $e_{sw} \equiv \ln(|\Psi_n(1-d)/\Psi_n^{[0]}(d)|)$ remains small we can replace the wavefunction Ψ_n by the the single-well wavefunction $\Psi_n^{[0]}$. A necessary condition is that $|V(1-d) - V^{[0]}(d)|/g \sim d^3/g$ remains small.

That this is also sufficient is analysed in full detail in the appendix of ref. 5. For any one-dimensional double-well problem we therefore find

$$\Delta E_n = 2g|\Psi_n^{[0]}(d)|^2\sqrt{2(V(1-d)-E_n)}\exp\Big(-\frac{1}{g}\int_{d-1}^{1-d}dz\ \sqrt{2(V(z)-E_n)}\Big)(1+err) \tag{49}$$

In the example under consideration, the total relative error $err=\mathcal{O}(g/d^2+d^3/g)$ is minimal if we choose $d=\hat{d}g^{\frac{2}{5}}$, thus demonstrating that errors can be kept under control. Let us emphasize though, that the actual relative error in the asymptotic expansion will in general be much smaller, since much of the error is due to conveniently approximating the full potential by the single-well potential in computing the wavefunction at the surfaces Σ_i.

Substituting $V(x)=(x^2-1)^2/8$ and $E_n=g(n+\frac{1}{2})(1+\mathcal{O}(\sqrt{g}))$ in eq. (49), we obtain (neglecting terms of higher order)

$$\begin{aligned}\Delta E_n &= 2gd|\Psi_n^{[0]}(d)|^2\exp[-(S-d^2)/g]\exp[(n+\tfrac{1}{2})T(d)]\\ &= \frac{2g\sqrt{2/\pi}}{n!}\Big(\frac{d^2\exp[T(d)]}{2g}\Big)^{(n+\frac{1}{2})}\exp(-S/g),\end{aligned} \tag{50}$$

where we have substituted the harmonic oscillator wavefunction

$$\Psi_n^{[0]}(x)=\frac{\exp(-\frac{d^2}{2g})H_n(d/\sqrt{g})}{\sqrt{2^n n!\sqrt{\pi g}}}. \tag{51}$$

The classical action S and the "tunnelling time" $T(d)$ (i.e. the time the euclidean classical solution requires to move from $x=d-1$ to $y=1-d$) are given by

$$S=\int_{-1}^{1}dz\sqrt{2V(z)}=2/3,\quad T(d)=\int_{d-1}^{1-d}dz\frac{1}{\sqrt{2V(z)}}=2\ln(2/d). \tag{52}$$

Substituting $T(d)$, the d dependence completely disappears, as is required for consistency, and we find the well-known result[2a]

$$\Delta E_n=\frac{4\sqrt{g}}{\sqrt{\pi}n!}(2/g)^n\exp(-S/g). \tag{53}$$

As a final example, we give the energy splitting for the ground state of the W-potential[5], $V(x)=||x|-1|$. The single-well wavefunction is in this case an Airy function, and if $v=1.018\cdots$ is the first zero of $dAi(-x)/dx$, we leave it as an exercise to verify that

$$\Delta E_0=\frac{(g/4)^{\frac{2}{3}}}{\pi v Ai(-v)^2}\exp\Big(-\frac{4\sqrt{2}}{3g}+\frac{2^{\frac{7}{6}}v}{g^{\frac{1}{3}}}\Big)(1+\mathcal{O}(g^{\frac{1}{3}})) \tag{54}$$

4. Explicit multi-dimensional examples

As we have seen in the previous section, the relevant quantity to evaluate is

$$<0|-\hbar M(E)|0>= \\ -\hbar\int_{\Sigma_1} d_{\Sigma_1}\mathbf{x}\int_{\Sigma_2} d_{\Sigma_2}\mathbf{y}\ \Psi_0^{(2)}(\mathbf{y})^*[\Sigma_1(\mathbf{y})]G^{(tr)}(\mathbf{y},\mathbf{x};E)[\Sigma_2(\mathbf{x})]\Psi_0^{(1)}(\mathbf{x}). \quad (55)$$

We compute $G^{(tr)}(\mathbf{y},\mathbf{x};E)$ with the semiclassical method, which involves stationary phase and/or steepest descent approximations (see the BOOK[8]). In essence one first computes $K_{eucl}(\mathbf{y},\mathbf{x};T)$ by expanding around the stationary point of the euclidean action (i.e. the classical path in the potential $-V$ that connects $\mathbf{x}$ and $\mathbf{y}$ in euclidean time T). In this expansion only quadratic fluctuations around the classical path are taken into account. Higher orders give relative errors that vanish with $\hbar$. The energy Green's function $G(\mathbf{y},\mathbf{x};E)$ is then evaluated by applying the stationary phase approximation to eq. (8), yielding (the dimension will be indicated by n)

$$G(\mathbf{y},\mathbf{x};E)=(\frac{1}{2\pi\hbar})^{\frac{1}{2}(n-1)}\sqrt{\det(J(\mathbf{y},\mathbf{x};E))}\exp(-W(\mathbf{y},\mathbf{x};E)/\hbar), \quad (56)$$

where J is square matrix of rank $n+1$

$$J=\begin{pmatrix} \frac{\partial^2 W}{\partial x_1\partial y_1} & \cdots & \frac{\partial^2 W}{\partial x_1\partial y_n} & \frac{\partial^2 W}{\partial x_1\partial E} \\ \vdots & \ddots & \vdots & \vdots \\ \frac{\partial^2 W}{\partial x_n\partial y_1} & \cdots & \frac{\partial^2 W}{\partial x_n\partial y_n} & \frac{\partial^2 W}{\partial x_n\partial E} \\ \frac{\partial^2 W}{\partial E\partial y_1} & \cdots & \frac{\partial^2 W}{\partial E\partial y_n} & \frac{\partial^2 W}{\partial E^2} \end{pmatrix}, \quad (57)$$

which accounts for the quantum fluctuations along the classical path in quadratic order. The Legendre transform of the action $S(\mathbf{y},\mathbf{x};T)$, that replaces E as indpendent parameter for T, is given by

$$W(\mathbf{y},\mathbf{x};E)=S(\mathbf{y},\mathbf{x};T)+E\cdot T. \quad (58)$$

Using the euclidean equations of motion

$$m\frac{d^2\mathbf{x}_i(t)}{dt^2}=\frac{\partial V}{\partial x_i}(\mathbf{x}(t)),\quad \mathbf{x}(0)=\mathbf{x},\quad \mathbf{x}(T)=\mathbf{y}, \quad (59)$$

one has

$$W(\mathbf{y},\mathbf{x};E)=\int_0^T dt\ |\dot{\mathbf{x}}(t)|\sqrt{2m(V(\mathbf{x}(t))-E)},\quad T=\frac{\partial W(\mathbf{y},\mathbf{x};E)}{\partial E}. \quad (60)$$

Let us define a moving orthonormal frame $\mathbf{e}^{(i)}(t)$ by parallel transport along the classical path, such that $\mathbf{e}^{(n)}(t)$ is tangent to it.

$$\mathbf{e}^{(n)}(t)=\dot{\mathbf{x}}(t)/|\dot{\mathbf{x}}(t)|,\quad \mathbf{e}^{(i)}(t)\cdot\mathbf{e}^{(j)}(t)=\delta_{ij}. \quad (61)$$

With respect to such a basis the matrix J takes a simpler form (the components of $\partial^2 W/\partial x_i \partial y_j$ tangent to the path will vanish, whereas the tangent component of $\partial^2 W/\partial x_i \partial E$ equals $\sqrt{\frac{1}{2}m/(V(\mathbf{x})-E)}$) and one has

$$\det(J)=\frac{m\det(\hat{J})}{2\sqrt{(V(\mathbf{x})-E)(V(\mathbf{y})-E)}}, \tag{62}$$

with $\hat{J}$ a square matrix of rank $n-1$

$$\hat{J}_{ij}=\mathbf{e}_k^{(i)}(0)\frac{\partial^2 W}{\partial x_k \partial y_\ell}\mathbf{e}_\ell^{(j)}(T). \tag{63}$$

By choosing Σ_i sufficiently far from the classically allowed region, the wave-function will have an asymptotic expansion of the form

$$\Psi_E^{(i)}(\mathbf{x})=A_E^{(i)}(\mathbf{x})\hbar^\beta\exp(-\phi_E^{(i)}(\mathbf{x})/\hbar) \tag{64}$$

and we can evaluate the surface integrals of eq. (55) by steepest descent. The stationary point $(\mathbf{x}_0,\mathbf{y}_0)$ is defined by minimizing

$$W(\mathbf{y},\mathbf{x};E)+\phi_E^{(1)}(\mathbf{x})+\phi_E^{(2)}(\mathbf{y}) \tag{65}$$

with respect to $\mathbf{x}\in\Sigma_1$ and $\mathbf{y}\in\Sigma_2$ (for sake of simplicity we will assume there is a *unique* minimum). We arrange our surfaces such that at $\mathbf{x}_0$ and $\mathbf{y}_0$ they are perpendicular to the associated tunnelling path (see figs. 2 and 3). In that case we can decompose

$$\mathbf{x}-\mathbf{x}_0=\sum_{i=1}^{n-1}\xi_i\mathbf{e}^{(i)}(0),\quad \mathbf{y}-\mathbf{y}_0=\sum_{i=1}^{n-1}\eta_i\mathbf{e}^{(i)}(T). \tag{66}$$

Expanding eq. (55) to second order in ξ and η, and performing the Gaussian integration gives

$$\begin{aligned}<0|\hbar M(E)|0>=\hbar\Big[4m^2(V(\mathbf{x}_0)-E)(V(\mathbf{y}_0)-E)\Big]^{\frac{1}{4}}\Psi_0^{(2)}(\mathbf{y}_0)^*\Psi_0^{(1)}(\mathbf{x}_0)\times\\ \exp(-W(\mathbf{y}_0,\mathbf{x}_0;E)/\hbar)\Lambda(\mathbf{y}_0,\mathbf{x}_0;E).\end{aligned} \tag{67}$$

Before defining Λ, first some remarks. We have implemented what was said below eq. (46) about the two-sided derivatives that occur in $[\Sigma_i]$, taking instead of $G^{(tr)}$ (which vanishes on Σ_i) a Green's function $G^{(e)}$ that is extend suitably inside the wells. Realizing that the final result is independent of the precise location of Σ_i is another way of seeing that the "velocities" have to match and that the two-sided derivative can be replaced by twice the derivative acting on the Green's function.

The method of images would give the same factor 2, but the above argument is more general. For the semiclassical result it would, nevertheless, be irrelevant whether we would use $G^{(e)}$ or $G^{(u)}$ (the construction of both was described in more detail in the previous section). Having said this we can return to the definition of Λ. It contains all Gaussian factors from the fluctuations around the tunnelling path and endpoints $\mathbf{x}_0, \mathbf{y}_0$. In one dimension we would thus have $\Lambda \equiv 1$ and eq. (67) reproduces the results of the previous section (compare eqs. (47), (48) and (49)). Explicitly we find

$$\Lambda(\mathbf{y}_0, \mathbf{x}_0; E) = (2\pi\hbar)^{\frac{1}{2}(n-1)} \sqrt{\det(\hat{J}(\mathbf{y}_0, \mathbf{x}_0; E)) / \det(\hat{I}(\mathbf{y}_0, \mathbf{x}_0; E))}, \tag{68}$$

where $\hat{I}$ is a square matrix of rank $2(n-1)$

$$\hat{I} = \begin{pmatrix} \hat{W}^{(1)} + \hat{\Phi}^{(1)} & \hat{J} \\ \hat{J}^t & \hat{W}^{(2)} + \hat{\Phi}^{(2)} \end{pmatrix}, \tag{69}$$

which is the Hessian of eq. (66) at $\mathbf{x}_0, \mathbf{y}_0$ in the directions perpendicular to the tunnelling path. The matrices $\hat{W}$ and $\hat{\Phi}$ are defined by

$$\hat{W}^{(1)}_{ij} = \frac{\partial^2 W}{\partial \xi_i \partial \xi_j}, \quad \hat{W}^{(2)}_{ij} = \frac{\partial^2 W}{\partial \eta_i \partial \eta_j}, \quad \hat{\Phi}^{(1)}_{ij} = \frac{\partial^2 \phi^{(1)}}{\partial \xi_i \partial \xi_j}, \quad \hat{\Phi}^{(2)}_{ij} = \frac{\partial^2 \phi^{(2)}}{\partial \eta_i \partial \eta_j}. \tag{70}$$

We will now show how Λ can be conveniently expressed in terms of the so-called stability equation. Let us define $\mathbf{q}(t) = \mathbf{x}(t) - \mathbf{x}_0(t)$ and $\mathbf{p}(t) = m\dot{\mathbf{q}}(t)$ for the deviation of the classical path $\mathbf{x}(t)$ from the path $\mathbf{x}_0(t)$ (with endpoints $\mathbf{x}_0$ and $\mathbf{y}_0$), which is used for evaluating $W(\mathbf{y}, \mathbf{x}; E)$. In particular both paths have an energy E and

$$m\dot{\mathbf{x}}(0) = -\frac{\partial W(\mathbf{y}, \mathbf{x}; E)}{\partial \mathbf{x}}, \quad m\dot{\mathbf{x}}(T) = \frac{\partial W(\mathbf{y}, \mathbf{x}; E)}{\partial \mathbf{y}}. \tag{71}$$

If $(\hat{q}_i(t), \hat{p}_i(t))$ are the components of $(\mathbf{q}(t), \mathbf{p}(t))$ with respect to the frame $\mathbf{e}^{(i)}(t)$, these equations, when expanded to first order in q give

$$\begin{aligned} \hat{p}_i(0) &= -\hat{W}^{(1)}_{ij} \hat{q}_j(0) - \hat{J}_{ij} \hat{q}_j(T), \\ \hat{p}_i(T) &= \quad \hat{W}^{(2)}_{ij} \hat{q}_j(T) + \hat{J}_{ji} \hat{q}_j(0). \end{aligned} \tag{72}$$

This allows us to solve $(\hat{q}_i(T), \hat{p}_i(T))$ to first order in q as a function of $(\hat{q}_i(0), \hat{p}_i(0))$

$$\begin{aligned} \hat{q}_i(T) &= \hat{A}_{ij} \hat{q}_j(0) + \hat{B}_{ij} \hat{p}_j(0), \\ \hat{p}_i(T) &= \hat{C}_{ij} \hat{q}_j(0) + \hat{D}_{ij} \hat{p}_j(0). \end{aligned} \tag{73}$$

with

$$\hat{A} = \hat{J}^{-1} \hat{W}^{(1)}, \quad \hat{B} = -\hat{J}^{-1}, \quad \hat{C} = \hat{J}^t - \hat{W}^{(2)} \hat{J}^{-1} \hat{W}^{(1)}, \quad \hat{D} = -\hat{W}^{(2)} \hat{J}^{-1} \tag{74}$$

and we leave it to the reader to check that

$$\Lambda = \frac{(2\pi\hbar)^{\frac{1}{2}(n-1)}}{\sqrt{\det(\hat{C} + \hat{D}\hat{\Phi}^{(1)} + \hat{\Phi}^{(2)}(\hat{A} + \hat{B}\hat{\Phi}^{(1)}))}}, \tag{75}$$

which makes apparent why we performed the above manipulations. Namely, suppose that we take

$$\hat{q}_i^{(b)}(0) = \varepsilon\delta_{ib}, \quad \hat{p}_i^{(b)}(0) = \varepsilon\hat{\Phi}_{ib}^{(1)}, \tag{76}$$

then eq. (73) shows us that Λ can equivalently be written as

$$\Lambda = \lim_{\varepsilon\to 0} \frac{(2\pi\hbar\varepsilon)^{\frac{1}{2}(n-1)}}{\sqrt{\det(\hat{p}_a^{(b)}(T) + \hat{\Phi}_{aj}^{(2)}\hat{q}_j^{(b)}(T))}}. \tag{78}$$

By solving the linearized fluctuation equations

$$m\frac{d^2q_i^{(b)}(t)}{dt^2} = \frac{\partial^2 V}{\partial x_i \partial x_j}(\mathbf{x}_0(t))q_j^{(b)}(t), \quad q_i^{(b)}(0) = e_i^{(b)}(0), \quad m\dot{q}_i^{(b)} = e_i^{(a)}\hat{\Phi}_{ab}^{(1)}, \tag{79}$$

we thus obtain an efficient method to compute Λ.

In the following, partly to avoid elaborate manipulations that tend to obscure the essential features, we assume a straight tunnelling path and a symmetric double well problem, allowing us to choose the orthonormal frame $\mathbf{e}^{(i)}(t)$ to be constant. In that case eq. (79) can be easily expressed in terms of the components with respect to this frame (see ref. 1 for details concerning the case of a curved tunnelling path, where an additional term proportional to the curvature will appear in the following equation)

$$m\frac{d^2\hat{q}_i^{(b)}(t)}{dt^2} = \hat{\Omega}_{ij}^2(t)\hat{q}_j(t), \quad \hat{q}_i^{(b)}(0) = \delta_{ib}, \quad m\dot{\hat{q}}_i^{(b)}(0) = \hat{\Phi}_{ib}, \tag{80}$$

with

$$m\hat{\Omega}_{ij}^2(t) = e_a^{(i)}\frac{\partial^2 V}{\partial x_a \partial x_b}(\mathbf{x}_0(t))e_b^{(j)}. \tag{81}$$

A special case arises when $\hat{\Omega}$ is bounded and

$$\max_t|\dot{\hat{\Omega}}(t)\hat{\Omega}^{-2}(t)| \equiv \varepsilon_{\rm ad} \tag{82}$$

will vanish as $\hbar \to 0$. In that case eq. (80) can be solved in the adiabatic limit (using the easily verified identities $\hat{\Phi} \equiv \hat{\Phi}^{(1)} = \hat{\Phi}^{(2)} = \hat{\Omega}(0) = \hat{\Omega}(T)$),

$$\Lambda = \frac{1}{\sqrt{\det(\frac{\hat{\Phi}}{\pi\hbar})}} \exp\Bigl(-\tfrac{1}{2}\int_0^T dt\ \mathrm{Tr}(\hat{\Omega})\Bigr). \tag{83}$$

Furthermore, as $\phi(\mathbf{x}) = \phi(\mathbf{x}_0) + \frac{1}{2}\hat{\Phi}_{ij}\xi_i\xi_j + \cdots$, the wavefunction can be decomposed in a transverse $n-1$-dimensional harmonic oscillator groundstate wavefunction

$$\chi(\xi) = \det(\frac{\hat{\Phi}}{\pi\hbar})^{\frac{1}{4}} \exp(-\tfrac{1}{2}\hat{\Phi}_{ij}\xi_i\xi_j/\hbar) \tag{84}$$

and a one-dimensional wavefunction $\psi(x)$ $(x \equiv \mathbf{x}\cdot\mathbf{e}^{(n)})$

$$\Psi(\mathbf{x}) = \psi(x)\chi(\xi). \tag{85}$$

It is now easily seen that in terms of this effectively one-dimensional wavefunction we find

$$\begin{aligned}\Delta E_0 =& 2\hbar\sqrt{2m(V(\mathbf{x}_0(0)) - E_0)} \exp\Big(-\frac{1}{\hbar}\int_0^T dt|\dot{\mathbf{x}}_0(t)|\sqrt{2m(V(\mathbf{x}_0(t)) - E_0)}\Big)\times \\ & |\psi_0(x_0(0))|^2 \exp\Big(-\tfrac{1}{2}\int_0^T dt\ \mathrm{Tr}(\hat{\Omega}(t))\Big).\end{aligned} \tag{86}$$

To the relevant order in $\hbar$ this is precisely equal to the one-dimensional result with a potential modified by the zero-point frequency of the transverse fluctuations (one-loop renormalization)

$$V_{eff}(z) = V(z\mathbf{e}^{(n)}) + \tfrac{1}{2}\hbar\mathrm{Tr}(\hat{\Omega}(z\mathbf{e}^{(n)})). \tag{87}$$

This result is of course not unexpected and would hardly justify the use of the PDX, were it not that there are many cases where the adiabatic approximation fails. This failure can be either close to the minima, such that the decomposition of the wavefunction in eq. (85) only holds in the classically forbidden region, or along the whole tunnelling path.

A failure of the first sort is particularly dramatic in the following two-dimensional Hamiltonain

$$H = -\frac{g^2}{2}(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}) + \frac{1}{2g^2}(x^2-1)^2y^2. \tag{88}$$

There is actually not even a classical barrier separating the two minima. Hence, at first sight it is not clear if the notion of minima makes sense. Yet, the particle moves in a potential with valleys that narrow if one moves further away from the points $(x, y) = (\pm 1, 0)$. It is the zero-point fluctuations in the direction transverse to the valleys that prevent the wavefunction from spreading (in terms of the classical trajectories, the particle will only run away to infinity if one aims its motion *exactly* along the valley). Therefore, the wavefunction will localize around $(x, y) = (\pm 1, 0)$ and the spectrum is discrete. Not too close to these points, along the valley the adiabatic approximation is certainly expected to be valid, but in the perturbative region it dramatically fails as the frequency for the transverse fluctuations vanishes at $(x, y) = (\pm 1, 0)$. However, it is sufficient to be able to use eq. (85) in a neighborhood of Σ_i. We simply compute the perturbative wavefunction in the wells numerically (the single-well potential $V^{[0]}(x,y)=2x^2y^2/g^2$ is non-integrable) to a sufficient accuracy to allow us to determine by projection the effective one-dimensional wavefunction $\psi(x)$. As we have the freedom to vary Σ_i within certain bounds one can check stability and consistency of the approximations. This type of analysis requires careful numerical manipulations as the perturbative wavefunction converges in the L^2 sense and only guarantees a good pointwise accuracy if the wavefunction is not too small, which tends to conflict with the requirement of establishing the asymptotics of the perturbative wavefunction. Nevertheless, this approach has been quite successful in specific cases as was described in detail in refs. 12 for a calculation in Quantum Chromodynamics. The results of a similar analysis for eq. (88) are described in appendix B of ref. 13. The expression for ΔE_0 has the same dependence on g as eq. (54); the various constants will of course be quite different. Finally, one needs to demonstrate that the error due to the failure of the adiabatic approximation in the perturbative regions can indeed be kept under control by suitably choosing Σ_i. An additional complication in this analysis is that the transition region overlaps with the classically allowed region, as the valley connects the two wells. This problem was analysed in depth in section 5 of ref. 5, which the reader should consult for details.

The second explicit example concerns the double-cone potential in three dimensions

$$H=-\frac{g^2}{2}\frac{\partial^2}{\partial\mathbf{x}^2}+\sqrt{(|x_1|-1)^2+x_2^2+x_3^2}. \tag{89}$$

The tunnelling path is obviously straight and situated along the the first axis. We choose $\mathbf{x}_0=(d{-}1,0,0)=-\mathbf{y}_0$ (see figure 3) and for the groundstate energy split we find

$$\Delta E_0=2g\Lambda(d)\sqrt{2d}|\Psi_0(\mathbf{x}_0)|^2\exp\Bigl(-\frac{1}{g}\int_{d-1}^{1-d}dz\sqrt{2(z-E_0)}\Bigr). \tag{90}$$

There are some common features this problem shares with all those cases where the potential is spherically symmetric near the minima. In that case the single-well wavefunction reduces to a one-dimensional problem (S_n is the surface area of a unit sphere in n-dimensions)

$$\Bigl(-\frac{g^2}{2}\frac{\partial^2}{\partial r^2}+V^{[0]}(r)-\frac{(n{-}1)(n{-}3)}{4r^2}\Bigr)\psi^{[0]}(r)=E^{[0]}\psi^{[0]}(r),\quad \Psi^{[0]}(\mathbf{x})=\frac{\psi^{[0]}(|\mathbf{x}|)}{\sqrt{S_n|\mathbf{x}|^{n-1}}}. \tag{91}$$

Thus, in the spherical single-well situation (the origin is shifted to one of the minima for the single-well quantities, as in the previous section), one finds

$$\Delta E_0=2g\Lambda(d)\sqrt{2V^{[0]}(d)}\frac{|\psi^{[0]}(d)|^2}{S_nd^{n-1}}\exp\Bigl(-\int_{d-1}^{1-d}dz\sqrt{2(V(z)-E_0)}\Bigr), \tag{92}$$

which, apart from the factor $\Lambda(d)/(S_nd^{n-1})$, coincides with the one-dimensional result. In the latter we have seen that the d-dependence cancels, such that it must be true that $\Lambda(d) \sim d^{n-1}$. For the case of a potential that is axially symmetric along the line connecting the two minima, this is proven independent of the shape of the potential in ref. 12 (between eqs. (7.17) and (7.27)).

For the case at hand we can therefore write $\Lambda(d) = gd^2\lambda$, where λ is a constant. One easily determines $\psi_0^{[0]}(d)$ in terms of the Airy function (compare eq. (54)) with a vanishing boundary condition at the origin. This fixes the single-well energy $E_0^{[0]}$ in terms of the first zero of $Ai(-r)$, $w = 2.338\cdots$ and one finds

$$\psi_0^{[0]}(r) = \frac{2^{\frac{1}{6}} Ai((2g^{-2})^{\frac{1}{3}} r - w)}{g^{\frac{1}{3}} Ai'(-w)}, \quad E_0^{[0]} = (g^2/2)^{\frac{1}{3}} w. \tag{93}$$

Inserting the appropriate asymptotic expansion of the Airy function eq. (92) yields

$$\begin{aligned} \Delta E_0 &= \frac{2^{\frac{2}{3}} \lambda g^{5/3}}{8\pi^2 Ai'(-w)^2} \exp\Big(-\frac{4\sqrt{2}}{3g} + \frac{2^{\frac{7}{6}} w}{g^{\frac{1}{3}}}\Big)(1 + \mathcal{O}(g^{\frac{1}{3}})), \\ \lambda &= 2\pi d^{-2}[\dot{q}(T) + \hat{\Phi}(d{-}1) q(T)]^{-1}. \end{aligned} \tag{94}$$

We have used that the fluctuations q in the two transverse directions decouple and both contribute the same amount to λ. Taking into account that

$$\hat{\Phi}(x) = \sqrt{2}\hat{\Omega}(x), \quad \hat{\Omega}(x) = |1 - |x||^{-\frac{1}{2}}, \quad \dot{x} = \sqrt{2|1 - |x||}, \tag{95}$$

Figure 3: The ingredients of the PDX for the double-cone potential, with Σ_i chosen such that one can apply the method of multiple images to compute $G^{(tr)}$, see eq. (44). (This is fig. 1 from ref. [5])

one accidentally finds a purely exponential solution for eq. (80)

$$q(t) = \exp\Big(\sqrt{2}\int_0^t dt\ \hat{\Omega}(x(t))\Big). \tag{96}$$

Despite its appearance, this does not coincide with the adiabatic approximation (which would have the form of eq. (96) without the factor $\sqrt{2}$). Explicitly

$$\lambda = \frac{\pi}{\sqrt{2}d^2}\exp\Big(-\sqrt{2}\int_{d-1}^{1-d} dx\ \frac{\hat{\Omega}(x)}{|\dot{x}|}\Big) = \frac{\pi}{\sqrt{2}}. \tag{97}$$

We end this section with an example where the failure of the adiabatic approximation for the transverse fluctuations will *not* be signaled by an inconsistent d-dependence, as would have occurred for the double-cone potential. To be specific let us consider the two-dimensional model

$$\begin{aligned} H &= -\frac{g^2}{2}\Big(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\Big) + \tfrac{1}{2}(x^2-1)^2 + \tfrac{1}{2}\hat{\Omega}^2(x)y^2, \\ \hat{\Omega}^2(x) &= \tfrac{1}{4} - \nu(\nu+1)(1-x^2), \quad k^2 \equiv 4\nu(\nu+1) > 1. \end{aligned} \tag{98}$$

Here we have (compare eq. (82))

$$\dot{x} = |1-x^2|, \quad \varepsilon_{\rm ad} = \frac{4\sqrt{3}k^2}{9(1-k^2)}. \tag{99}$$

The adiabatic approximation requires $\varepsilon_{\rm ad}$ to vanish as $g \to 0$, which means that k needs to vanish in this limit. However, in that case the potential is separable. Still, one would expect the adiabatic approximation to be reasonable, as long as k is not too big. It should be stressed that the error one thus makes will not vanish as $g \to 0$ and the adiabatic approximation will *not* give the correct asymptotic expansion for the energy split.

We have devised eq. (98) such that the stability or fluctuation equation can be solved exactly. Exchanging x for t as independent variable in eq. (80) we find

$$\begin{aligned} &(1-x^2)\partial_x^2 q(x) - 2x\partial_x q(x) + \Big(\nu(\nu+1) - \frac{\mu^2}{1-x^2}\Big)q(x) = 0, \\ &\mu = \tfrac{1}{2}, \quad q(d{-}1) = 1, \quad \partial_x q(d{-}1) = \frac{1}{4d}(1+\mathcal{O}(d)). \end{aligned} \tag{100}$$

This is precisely the Legendre equation with $\mu = \frac{1}{2}$, yielding a particularly simple solution for q in terms of the variable θ

$$q(\theta) = \frac{\sin((\nu+\frac{1}{2})(\theta+\alpha))}{\sin((\nu+\frac{1}{2})(\theta_0+\alpha))}\sqrt{\frac{\sin\theta_0}{\sin\theta}}, \quad x = -\cos\theta, \quad 1-\cos\theta_0 = d. \tag{101}$$

This is chosen so as to satisfy $q(\theta_0)=1$. Using

$$\partial_\theta q(\theta)=\{(\nu+\tfrac{1}{2})\cot((\nu+\tfrac{1}{2})(\theta+\alpha))-\tfrac{1}{2}\cot(\theta)\}q(\theta), \tag{102}$$

one easily verifies, by imposing the boundary condition for the derivative on q, that $\alpha=\mathcal{O}(\theta_0^3)$. Substituting q in the equation that determines Λ we obtain

$$\Lambda=\frac{\sqrt{2\pi g}}{\sqrt{\sin\theta_0\partial_\theta q(\pi-\theta_0)+\hat{\Omega}(\theta_0)q(\pi-\theta_0)}}=\sqrt{\frac{(2\nu+1)\pi g\sqrt{2d}}{\cos(\nu\pi)}}(1+\mathcal{O}(\sqrt{d})), \tag{103}$$

whereas the adiabatic approximation, eq. (83), can be seen to give

$$\Lambda_{\rm ad}=[2d\pi^2g^2(1-k)^{1-k}(1+k)^{1+k}]^{\frac{1}{4}}, \tag{104}$$

which deviates from eq. (103) at second order in ν. Nevertheless, numerically the adiabatic approximation tends to be quite accurate, e.g. at $\nu=\frac{1}{8}$, the error is only 7 per mille. It is left as an exercise for the reader to check that

$$\Delta E_0=8\sqrt{\frac{2\nu+1}{\cos(\nu\pi)}}\sqrt{\frac{2g}{\pi}}\exp(-\frac{4}{3g}). \tag{105}$$

Also useful to check is that at $\nu=0$ this agrees with eq. (53) after an appropriate rescaling.

5. Supersymmetric quantum mechanics

In this section we wish to discuss the application of the PDX to a one-dimensional tunnelling problem in supersymmetric quantum mechanics. We will first briefly make a few remarks motivating the general interest in this problem. Readers interested only in the bosonic formulation should not read between the lines, but between eq. (110) and eq. (124).

Tunnelling calculations in supersymmetric theories have played an important role in particle theory in an attempt to spontaneously break the symmetry[14]. These attempts have been frustrated for topological reasons, whose understanding has led to the appealing interpretation of tunnelling in supersymmetric quantum mechanics, defined on a compact manifold, in terms of the Morse theory for that manifold[15]. It gives an explicit model of the De Rham cohomology in terms of the gradient lines (i.e. the tunnelling paths) for the Morse function. It has been a precursor for the recently discovered topological field theories[16], where the BRST symmetry plays the role of the supersymmetry and the (equivariant) BRST cohomology the role of the De Rham cohomology. For a pedagogical review that emphasizes the cohomological aspects and their relation to tunnelling we refer to ref. 17.

Supersymmetry relates the bosonic and fermionic fluctuations and as they give opposite contributions to the amplitudes, the prefactor in the tunnelling calculations is expected to be trivial. In the cohomological analysis this prefactor is assumed to be a combination of integers (counting the various instantons that can occur with an appropriate sign). This, however, can not be correct in the light of the results obtained in ref. 6, where the supersymmetric instanton calculation was performed by very carefully prescribing the integration over the Grassman variables that occur in the path integral. Nevertheless, these results show that the prefactor only depends on the curvature of the superpotential at its critical points, where the wavefunction will be localized, a result we expect also to be valid in more than one dimension. This can be shown to imply that the relevant cohomology remains unaffected, as was to be expected. One could of course have appealed to the general theory for the gradient line formulation of Morse theory, but the upshot of using supersymmetric quantum mechanics is that it provides an explicit construction of such a theory.

The Hamiltonian for one-dimensional supersymmetric quantum mechanics is formulated in terms of an x-dependent two-component spinor field, and is conveniently expressed in terms of the supercharge (i.e. the supersymmetry generator)

$$Q = -i(g\partial_x - \partial_x \mathcal{V}(x))\sigma_-, \tag{106}$$

where $\sigma_- = \frac{1}{2}(\sigma_1 - i\sigma_2)$ (σ_k are the Pauli-matrices) and $\mathcal{V}$ is the so-called superpotential. The Hamiltonian is now given by

$$H = \tfrac{1}{2}(Q^\dagger + Q)^2 = \tfrac{1}{2}\{Q^\dagger, Q\} \tag{107}$$

and is obviously positive definite and commuting with Q and $Q^\dagger$. We will not dwell on the fermionic content of the theory here. We can afford doing so in one dimension, since the Hamiltonian takes a block diagonal form

$$H = \begin{pmatrix} H_+ & 0 \\ 0 & H_- \end{pmatrix}, \quad H_\pm = -\tfrac{1}{2}g^2\partial_x^2 + \tfrac{1}{2}\Big(\frac{d\mathcal{V}(x)}{dx}\Big)^2 \pm \frac{g}{2}\Big(\frac{d^2\mathcal{V}(x)}{dx^2}\Big). \tag{108}$$

Both one-component one-dimensional Hamiltonians $H_\pm$ have identical spectra due to the supersymmetry. Also, there is always an exact zero-energy state for $H_\pm$

$$\Psi_0^\pm(x) = \exp(\pm\mathcal{V}(x)/g), \tag{109}$$

which is, however, not always normalizable. (The zero-energy states need not to occur in pairs, as they are annihilated by the supercharge.) Obviously, the classical vacua occur at the critical points of the the superpotential $\mathcal{V}$. The g-dependence of the potential in eq. (108) can be understood as the quantum correction one gets by integrating out the fermionic degrees of freedom, which in this one-dimensional case is *exact*.

To be specific, we consider a one-dimensional Hamiltonain defined on the circle $[0,2\pi]$, derived from a superpotential $\mathcal{V}(x)=2\cos^2 x$, such that

$$H=-\tfrac{1}{2}g^2\partial_x^2+2\sin^2(2x)-2g\cos(2x). \tag{110}$$

The potential $V(x)=2(\sin^2(2x)-g\cos(2x))$ has minima at $x=0$ and $x=\pi$ (see figure 4) and we want to compute the groundstate energy split between the even and odd states with respect to reflection in $\frac{1}{2}\pi$. Due to the special form of this potential we know the exact groundstate wavefunction ($E=0$, compare eq. (109))

$$\Psi_0(x)=\frac{\exp(\cos(2x)/g)}{\sqrt{2\pi I_0(2g)}}, \tag{111}$$

which is properly normalized in terms of the modified Bessel function I_0, although we will not require its exact form. Due to the 2π periodicity there are *two* tunnelling paths connecting 0 and π, one will go clockwise, the other counterclockwise. Due to the symmetry they contribute an equal amount to the matrix element $<0|M(0)|0>$ and our formula for ΔE_0 will contain an extra factor 2, where from now on we concentrate on the tunnelling in the interval $[0,\pi]$.

The interesting feature of this problem is that the classical path will spent a time proportional to $\ln(g)$ around $x=\frac{1}{2}\pi$, despite its location in the classically forbidden region, and one can expect the WKB approximation to break down. This break down is nevertheless rather subtle. Naively applying our one-dimensional result of eq. (49) would give

$$\Delta E_0^{naive}=4g\sqrt{2V(d)}|\Psi_0(d)|^2\exp\Bigl(-\frac{1}{g}\int_d^{\pi-d}dx\sqrt{2V(x)}\Bigr). \tag{112}$$

The treacherous part is that, although requiring due care, the WKB integral can be properly evaluated, yielding a result in which the d-dependence neatly cancels, but nevertheless giving a result that is off by a factor $\sqrt{e/\pi}$.

We will demonstrate how the PDX allows for an elegant way of doing the calculation correctly. Rather than dividing the circle in the well regions $[-d,d]$ and $[\pi-d,\pi+d]$, we add two more well regions, $[\frac{1}{2}\pi-d,\frac{1}{2}\pi+d]$ and $[\frac{3}{2}\pi-d,\frac{3}{2}\pi+d]$. The four "well" Green's functions $G_w^{(i)}$ are defined on resp. $[\frac{1}{2}\pi(i-1)+d,\frac{1}{2}\pi(i+1)-d]$ and the four transition Green's functions $G_{tr}^{(i)}$ are defined on $[\frac{1}{2}\pi i+d,\frac{1}{2}\pi(i+1)-d]$, all taken to vanish on the boundaries of these domains. We leave it to the reader's ingenuity to show that the PDX construction in this case yields

$$\begin{aligned}\Delta E_0=4g|\Psi_0^{(3)}(x_4)^*\frac{g^2}{4}\frac{\partial^2}{\partial x_4\partial x_3}\Bigl[G_{tr}^{(2)}(x_4,x_3;0)\Bigr]G_w^{(2)}(x_3,x_4;0)\times\\ \frac{g^2}{4}\frac{\partial^2}{\partial x_1\partial x_2}\Bigl[G_{tr}^{(1)}(x_2,x_1;0)\Bigr]\Psi_0^{(1)}(x_1)|,\end{aligned} \tag{113}$$

where $x_1 = d$, $x_2 = \frac{1}{2}\pi - d$, $x_3 = \frac{1}{2}\pi + d$ and $x_4 = \pi - d$. Now, however, it is entirely justified to apply the standard WKB approximation for the two transition Green's function and the result simplifies to

$$\Delta E_0 = 4g\sqrt{2V(d)}|\Psi_0^{(1)}(d)|^2 \exp\Bigl(-\frac{2}{g}\int_d^{\frac{1}{2}\pi-d} dx\sqrt{2V(x)}\Bigr)\times \\ \sqrt{2V(\tfrac{1}{2}\pi - d)}|G_w^{(2)}(\tfrac{1}{2}\pi + d, \tfrac{1}{2}\pi - d; 0)|, \tag{114}$$

where we have used the symmetry of V with respect to $\frac{1}{2}\pi$ to equate the contribution of the two transition Green's functions. Therefore, eq. (112) could only be correct if

$$\exp(-S_w/g) =?= \sqrt{2V(\tfrac{1}{2}\pi - d)}|G_w^{(2)}(\tfrac{1}{2}\pi + d, \tfrac{1}{2}\pi - d; 0)|, \tag{115}$$

where

$$S_w \equiv \int_{\frac{1}{2}\pi-d}^{\frac{1}{2}\pi+d} dx\sqrt{2V(x)} = 4\int_0^d dx\sqrt{\sin^2(2x) + g\cos(2x)}, \\ S_{tr} \equiv \int_d^{\frac{1}{2}\pi-d} dx\sqrt{2V(x)} = 2\int_d^{\frac{1}{4}\pi} dx\Bigl(\sqrt{\sin^2(2x) + g\cos(2x)} + \\ \sqrt{\sin^2(2x) - g\cos(2x)}\Bigr). \tag{116}$$

This yields, after writing

$$S_w = 4\int_0^d dx\sqrt{(r_+ + 2\sin^2 x)}\sqrt{(2\cos^2 x + r_-)}, \quad r_\pm = \sqrt{1 + \tfrac{1}{4}g^2} \pm \tfrac{1}{2}g \tag{117}$$

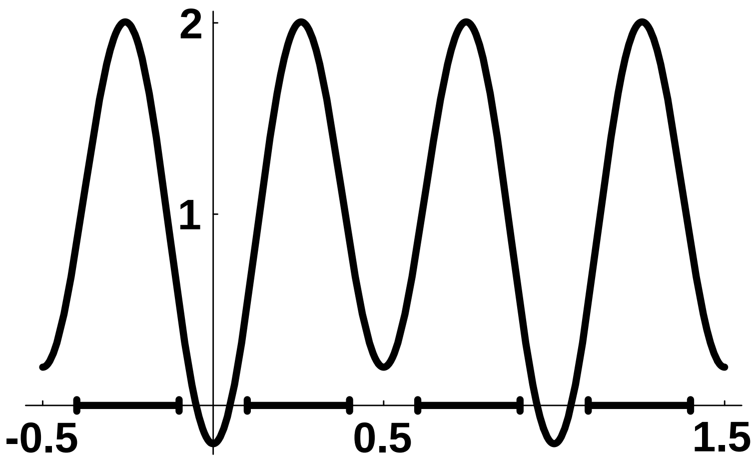

Figure 4: The potential for the one-dimensional supersymmetric quantum mechanics problem, eq. (110) (x is plotted horizontally in units of π, whereas g=0.1). Indicated are the positions of the points x_i that define the various wells and transition regions (the thick segments) appearing in eq. (113).

and expanding in r_-

$$S_w = 4d^2 + \tfrac{1}{2}g + \tfrac{1}{2}g\ln(16d^2/g) + \mathcal{O}(gd^2, d^4), \quad S_{tr} = 2 - 4d^2 + \mathcal{O}(gd^2, d^4). \quad (118)$$

As in section 3 (see the discussion around eq. (49)) we choose d such that $g/d^2 + d^3/g$ remains small, e.g. $d = \hat{d}g^{\frac{2}{5}}$. This allows us to use the harmonic approximation for the potential in *all* well regions. The relevant harmonic potential has $\omega = 4$ and we can therefore substitute for $\Psi_0^{(1)}$ the harmonic oscillator wavefunction

$$|\Psi_0^{(1)}|^2 = \frac{\exp(-4d^2/g)}{\sqrt{\frac{1}{2}\pi g}} \quad (119)$$

and for $G_w^{(2)}$ the harmonic oscillator Green's function

$$G_w^{(2)}(\tfrac{1}{2}\pi + y, \tfrac{1}{2}\pi + x; E) = \tfrac{1}{2}G(2y/\sqrt{g}, 2x/\sqrt{g}; \tfrac{1}{4}E/g - \tfrac{1}{2})/\sqrt{g}, \quad (120)$$

where G is the energy Green's function for the "unit" harmonic oscillator ($\hbar = m = \omega = 1$). Using the well-known result[7] for the euclidean propagator of the "unit" harmonic oscillator

$$K_{eucl}(y, x; t) = \frac{1}{\sqrt{2\pi\sinh(t)}}\exp\Bigl(\frac{2xy - (x^2 + y^2)\cosh(t)}{2\sinh(t)}\Bigr), \quad (121)$$

we obtain (see eq. (8))

$$\begin{aligned} G(x, -x; -\tfrac{1}{2}) &= \frac{1}{\sqrt{\pi}}\int_0^\infty dt\ \frac{e^{-t}}{\sqrt{1 - e^{-2t}}}\exp(-x^2\coth(\tfrac{1}{2}t)) \\ &= \frac{e^{-x^2}}{2\sqrt{\pi}x^2}\int_0^\infty du\ \frac{e^{-u}}{(1 + \frac{1}{2}ux^{-2})\sqrt{1 + ux^{-2}}}, \end{aligned} \quad (122)$$

where $u = 2x^2e^{-t}/(1 - e^{-t})$ provides a change of variables in which the asymptotic expansion of the integral becomes straightforward. Combining this result with eq. (120) gives us the last ingredient

$$G_w^{(2)}(\tfrac{1}{2}\pi + d, \tfrac{1}{2}\pi - d; 0) = \sqrt{\frac{g}{\pi}}\frac{\exp(-4d^2/g)}{16d^2}. \quad (123)$$

We thus find that eq. (115) is not satisfied and that there is a mismatch of a factor $\sqrt{e/\pi}$; eq. (112) *is indeed too naive.* Combining all the results we finally obtain

$$\Delta E_0 = \frac{8g}{\pi}e^{-4/g} = 4g\frac{|\mathcal{V}''(0)|}{2\pi}\exp(-2|\mathcal{V}(\tfrac{1}{2}\pi) - \mathcal{V}(0)|). \quad (124)$$

Formulated in terms of the superpotential $\mathcal{V}(x) = 2\cos^2(x)$, this result is *universal* and agrees with the supersymmetric instanton results of Salomonson and Van Holten[6].

The comparison with ref. 6 needs some further study, which is interesting in its own right, as the analysis there was based on the case that the superpotential $\mathcal{V}$ had only two critical points, say x_1 is a local maximum and x_2 a local minimum. These critical points give rise to two perturbative zero-energy eigenstates $|n_i>$, localized around x_i (supersymmetric harmonic oscillator wavefunctions) and using fermionic zero-modes and chirality, the supersymmetric instanton analysis allows one to show that $< n_i|Q|n_j >= A\sigma^-_{ij}$. The Hamiltonian, when expressed in the basis $|n_i>$, is now easily found to be $H_{ij} = \frac{1}{2}(Q_{ij} + Q^\dagger_{ij})^2 = \frac{1}{2}|A|^2\delta_{ij}$. Note that this implies that supersymmetry is spontaneously broken unless $A = 0$. The latter will be the case if $\mathcal{V}$ is defined on the circle and has only two extrema. In that case A will receive a contribution from a clockwise *and* a counterclockwise tunnelling, equal in magnitude, but opposite in sign. It is a manifestation of the trivial cohomology of the circle.

For our choice of $\mathcal{V}(x) = 2\cos^2(x)$ there are four extrema, leading to four perturbative zero-energy wavefunctions $|n_i>$, respectively localized around $x = 0$, $x = \frac{1}{2}\pi$, $x = \pi$ and $x = \frac{3}{2}\pi$. With respect to this basis the general formulation of supersymmetric tunnelling[15,17] allows one to show that

$$Q = \begin{pmatrix} 0 & 0 & 0 & 0 \\ A & 0 & A & 0 \\ 0 & 0 & 0 & 0 \\ -A & 0 & -A & 0 \end{pmatrix}. \qquad (125)$$

The resulting Hamiltonian $H = \frac{1}{2}(Q + Q^\dagger)^2$ thus obtained was independently derived by J. Verbaarschot[18], using techniques described in ref. 19. It can be easily diagonalized yielding the eigenvalues 0 and $2|A|^2$, both with multiplicity 2. The value of A can be directly taken from the supersymmetric instanton computation[6], $|A| = \sqrt{(g|\mathcal{V}"(0)|/\pi)}\exp(-|\mathcal{V}(\frac{1}{2}\pi) - \mathcal{V}(0)|)$, thereby reproducing eq. (124). Note that the two-fold degeneracy agrees with the fact that we have to add the spectrum of H_-, as eq. (110) only represents the H_+ part. That the spectrum of H_- is identical to that of H_+ can in this case be seen by simply shifting x over $\frac{1}{2}\pi$.

6. Conclusions

These notes should have convinced you about the usefulness of the Path Decomposition Expansion. We stress again that, although its interpretation in terms of path integrals is the most natural one, the Green's function formulation is more rigorous and also tells one how to use it in the presence of gauge fields (e.g. a magnetic field, just to please Devreese). We have predominantly concentrated on problems concerning tunnelling between two degenerate minima, discussing in detail a wide range of examples. The examples have been kept as simple as possible in order to illustrate the salient features. For many applications in practical situations we refer the reader to ref. 1, where mainly applications in condensed matter physics were discussed and ref. 12, where the PDX was applied to field theory.

Writing these lecture notes, and that is a useful aspect of such an endeavour, has triggered me to clean up quite a number of 'nasty little' problems I would have otherwise left lying around. They are: *i*. The rigorous proof of the PDX using the Green's function technique. *ii*. The correct evaluation of the energy dependent Hamiltonian $\mathcal{H}$ for the tunnelling problem. *iii*. Demonstrating the subtle failure of the adiabatic approximation for the transverse fluctuations, despite the quadratic behaviour of the potential, where ever it matters. *iv*. Obtaining the energy split for one-dimensional supersymmetric quantum mechanics using the PDX, thereby reproducing the supersymmetric instanton calculations. Hopefully including them enhances, rather than diminishes the pedagogical value of these notes.

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