3
The Symmetric Double Well

In this chapter we will consider in detail a simple quantum mechanical system where "instantons", critical points of the classical Euclidean action, can be used to uncover non-perturbative information about the energy levels and matrix elements. We will also explicitly see the use of the particular matrix element (2.27) that we consider. The model we will consider has the classical Euclidean action

$$S_E[z(\tau)] = \int_{-\frac{\beta}{2}}^{\frac{\beta}{2}} d\tau \left(\frac{1}{2}(\dot{z}(\tau))^2 + V(z(\tau)) \right). \tag{3.1}$$

We choose for convenience the domain $[-\frac{\beta}{2}, \frac{\beta}{2}]$ and we will choose the potential explicitly later. We will always have in mind that $\beta \to \infty$, thus if β is considered finite, it is to be treated as arbitrarily large. The potential, for now, is simply required to be a symmetric double well potential, adjusted so that the energy is equal to zero at the bottom of each well, located at $\pm a$, as depicted in Figure 3.1.

3.1 Classical Critical Points

The critical points of the action, Equation (3.1), are achieved at solutions of the equations of motion

$$\left. \frac{\delta S_E[z(\tau)]}{\delta z(\tau')} \right|_{z(\tau')=\bar{z}(\tau')} = -\ddot{\bar{z}}(\tau') + V'(\bar{z}(\tau')) = 0. \tag{3.2}$$

We assume $\bar{z}(\tau)$ satisfies Equation (3.2). Then writing $z(\tau) = \bar{z}(\tau) + \delta z(\tau)$ and expanding in a Taylor series, we find

$$S_E[z(\tau)] = S_E[\bar{z}(\tau)] + \frac{1}{2} \int d\tau' d\tau'' \left. \frac{\delta^2 S_E[z(\tau)]}{\delta z(\tau')\delta z(\tau'')} \right|_{z(\tau)=\bar{z}(\tau)} \delta z(\tau')\delta z(\tau'') + \cdots, \tag{3.3}$$

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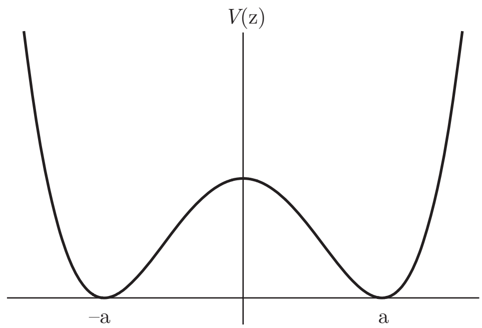

Figure 3.1. A symmetric double well potential with minima at $\pm a$

where we note that the first-order variation is absent as the equations of motion, Equation (3.2), are satisfied. The second-order variation is given by

$$\left.\frac{\delta^2 S_E[z(\tau)]}{\delta z(\tau')\delta z(\tau'')}\right|_{z(\tau)=\bar{z}(\tau)} = \left(-\frac{d^2}{d\tau'^2} + V''(\bar{z}(\tau')\right)\delta(\tau' - \tau''). \tag{3.4}$$

Then we have

$$S_E[z(\tau)] = S_E[\bar{z}(\tau)] + \frac{1}{2}\int_{-\frac{\beta}{2}}^{\frac{\beta}{2}} d\tau \delta z(\tau)\left(-\frac{d^2}{d\tau^2} + V''(\bar{z}(\tau))\right)\delta z(\tau) + \cdots . \tag{3.5}$$

We can expand $\delta z(\tau)$ in terms of the complete orthonormal set of eigenfunctions $z_n(\tau)$ of the hermitean operator entering in the second-order term

$$\left(-\frac{d^2}{d\tau^2} + V''(\bar{z}(\tau))\right) z_n(\tau) = \lambda_n z_n(\tau), \quad n = 0, 1, 2, 3, \cdots, \infty \tag{3.6}$$

supplied with the boundary conditions

$$z_n(-\frac{\beta}{2}) = z_n(\frac{\beta}{2}) = 0. \tag{3.7}$$

Completeness implies

$$\sum_{n=0}^{\infty} z_n(\tau) z_n(\tau') = \delta(\tau - \tau') \tag{3.8}$$

while orthonormality gives

$$\int_{-\frac{\beta}{2}}^{\frac{\beta}{2}} d\tau z_n(\tau) z_m(\tau) = \delta_{nm}. \tag{3.9}$$

Thus expanding

$$\delta z(\tau) = \sum_{n=0}^{\infty} c_n z_n(\tau) \tag{3.10}$$

we find

$$S_E[z(\tau)] = S_E[\bar{z}(\tau)] + \frac{1}{2}\sum_{n=0}^{\infty} \lambda_n c_n^2 + \mathrm{o}(c_n^3) \tag{3.11}$$

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using the orthonormality Equation (3.9) of the $z_n(\tau)$'s.

3.2 Analysis of the Euclidean Path Integral

The original matrix element that we wish to study, Equation (2.32), is given by

$$\langle y|e^{-\frac{\beta}{\hbar}\hat{h}(\hat{X},\hat{P})}|x\rangle = \langle\bar{z}(\beta/2)|e^{-\frac{\beta}{\hbar}\hat{h}(\hat{X},\hat{P})}|\bar{z}(-\beta/2)\rangle, \tag{3.12}$$

as we have not yet picked the boundary conditions on $\bar{z}(\pm\beta/2)$. Then we get

$$\begin{aligned}\langle\bar{z}(\beta/2)|e^{-\frac{\beta}{\hbar}\hat{h}(\hat{X},\hat{P})}|\bar{z}(-\beta/2)\rangle &= \mathcal{N}\int\mathcal{D}z(\tau)e^{-\frac{1}{\hbar}\left(S_E[\bar{z}(\tau)]+\frac{1}{2}\sum_{n=0}^{\infty}\lambda_n c_n^2+\mathrm{o}(c_n^3)\right)}\\ &= e^{-\frac{S_E[\bar{z}(\tau)]}{\hbar}}\mathcal{N}\int\mathcal{D}z(\tau)e^{-\frac{1}{\hbar}\left(\sum_{n=0}^{\infty}\frac{1}{2}\lambda_n c_n^2+\mathrm{o}(c_n^3)\right)}.\end{aligned} \tag{3.13}$$

Now we will begin to define the path integration measure as

$$\mathcal{D}z(\tau)\to\prod_{n=0}^{\infty}\frac{dc_n}{\sqrt{2\pi\hbar}}, \tag{3.14}$$

integrating over all possible values of the c_n's as a reasonable way of integrating over all paths. The factor of $\sqrt{2\pi\hbar}$ in the denominator is purely a convention and is done for convenience as we shall see; any difference in the normalization obtained this way can be absorbed into the still undefined normalization constant, $\mathcal{N}$. Then the expression for the matrix element in Equation (3.13) becomes

$$\langle\bar{z}(\beta/2)|e^{-\frac{\beta}{\hbar}\hat{h}(\hat{X},\hat{P})}|\bar{z}(-\beta/2)\rangle = e^{-\frac{S_E[\bar{z}(\tau)]}{\hbar}}\mathcal{N}\prod_{n=0}^{\infty}\int\frac{dc_n}{\sqrt{2\pi\hbar}}e^{-\frac{1}{\hbar}\left(\sum_{n=0}^{\infty}\frac{1}{2}\lambda_n c_n^2+\mathrm{o}(c_n^3)\right)}. \tag{3.15}$$

Scaling $c_n = \tilde{c}_n\sqrt{\hbar}$ gives for the right-hand side

$$\begin{aligned}&= e^{-\frac{S_E[\bar{z}(\tau)]}{\hbar}}\mathcal{N}\prod_{n=0}^{\infty}\int\frac{d\tilde{c}_n}{\sqrt{2\pi}}e^{-\left(\frac{1}{2}\lambda_n\tilde{c}_n^2+\mathrm{o}(\hbar)\right)}\\ &= e^{-\frac{S_E[\bar{z}(\tau)]}{\hbar}}\mathcal{N}\prod_{n=0}^{\infty}\left(\frac{1}{\sqrt{\lambda_n}}(1+\mathrm{o}(\hbar))\right).\end{aligned} \tag{3.16}$$

This infinite product of eigenvalues for the operators which arise typically does not converge. We will address and resolve this difficulty later and, assuming that it is so done, we formally write "det" for the product of all the eigenvalues of the operator. This yields the formula

$$\langle\bar{z}(\beta/2)|e^{-\frac{\beta}{\hbar}\hat{h}(\hat{X},\hat{P})}|\bar{z}(-\beta/2)\rangle = e^{-\frac{S_E[\bar{z}(\tau)]}{\hbar}}\left(\mathcal{N}\det^{-\frac{1}{2}}\left[-\frac{d^2}{d\tau^2}+V''(\bar{z}(\tau))\right](1+\mathrm{o}(\hbar))\right). \tag{3.17}$$

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Thus we see the matrix element has a non-perturbative contribution in $\hbar$ coming from the exponential of the value of the classical action at the critical point divided by $\hbar$, $e^{-\frac{S_E[\bar{z}(\tau)]}{\hbar}}$, multiplying the yet undefined normalization and determinant and an expression which has a perturbative expansion in positive powers of $\hbar$.

3.3 Tunnelling Amplitudes and the Instanton

To proceed further we have to be more specific. We shall consider the following matrix elements

$$\langle \pm a|e^{-\frac{\beta}{\hbar}\hat{h}(\hat{X},\hat{P})}|a\rangle = \langle \mp a|e^{-\frac{\beta}{\hbar}\hat{h}(\hat{X},\hat{P})}|-a\rangle. \tag{3.18}$$

The equality of these matrix elements is easily obtained here by using the assumed parity reflection symmetry of the Hamiltonian,

$$\begin{aligned}\langle x|e^{-\frac{\beta}{\hbar}\hat{h}(\hat{X},\hat{P})}|y\rangle &= \langle x|\mathfrak{P}\mathfrak{P}e^{-\frac{\beta}{\hbar}\hat{h}(\hat{X},\hat{P})}\mathfrak{P}\mathfrak{P}|y\rangle \\ &= \langle -x|\mathfrak{P}e^{-\frac{\beta}{\hbar}\hat{h}(\hat{X},\hat{P})}\mathfrak{P}|-y\rangle \\ &= \langle -x|e^{-\frac{\beta}{\hbar}\hat{h}(\hat{X},\hat{P})}|-y\rangle,\end{aligned} \tag{3.19}$$

where $\mathfrak{P}$ is the parity operator which satisfies $\mathfrak{P}^2 = 1$, $\mathfrak{P}|x\rangle = |-x\rangle$ and $[\mathfrak{P},\hat{h}(\hat{X},\hat{P})] = 0$.

The equation which $\bar{z}(\tau)$ satisfies is

$$-\ddot{\bar{z}}(\tau) + V'(\bar{z}(\tau)) = 0, \tag{3.20}$$

which is exactly the equation of motion for a particle in real time moving in the reversed potential $-V(z)$, as in Figure 3.2. Because of the matrix elements that we are interested in, Equation (3.18), the corresponding classical solutions are those which start at and return to either $\pm a$ or those that interpolate between

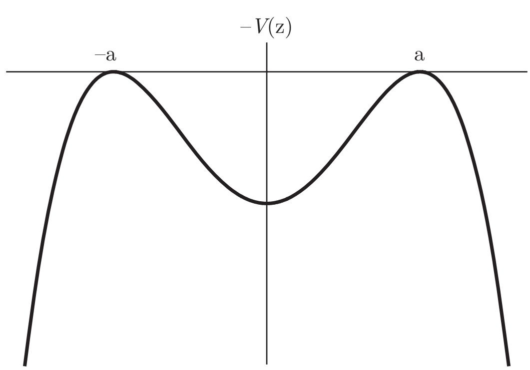

Figure 3.2. Inverted double well potential for $\bar{z}(\tau)$

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$\pm a$ and $\mp a$, and each in time β. The trivial solutions

$$\bar{z}(\tau) = \pm a \tag{3.21}$$

satisfy the first condition while the second condition can be obtained by integrating Equation (3.20). Straightforwardly,

$$\ddot{\bar{z}}(\tau)\dot{\bar{z}}(\tau) = V'(\bar{z}(\tau))\dot{\bar{z}}(\tau), \tag{3.22}$$

which implies

$$\dot{\bar{z}}(\tau) = \sqrt{2V(\bar{z}(\tau)) + c^2}, \tag{3.23}$$

where c is an integration constant. Integrating one more time and choosing the solution that interpolates from $-a$ to a, we get

$$\int_{-a}^{\bar{z}(\tau)} \frac{d\bar{z}}{\sqrt{2V(\bar{z}) + c^2}} = \int_{-\frac{\beta}{2}}^{\tau} d\tau = \tau + \frac{\beta}{2} \tag{3.24}$$

and c is determined by

$$\int_{-a}^{a} \frac{d\bar{z}}{\sqrt{2V(\bar{z}) + c^2}} = \beta. \tag{3.25}$$

We note that this last Equation (3.25) does not depend on the details of the solution, but only on the fact that it must interpolate from $-a$ to a. Obviously from Equation (3.23), c is the initial velocity. The initial velocity is not arbitrary, the solution must interpolate from $-a$ to a in Euclidean time β, and Equation (3.25) implicitly gives c as a function of β. There is no solution that starts with vanishing initial velocity but interpolates between $\pm a$ in finite time β; vanishing initial velocity requires infinite time.

As $\beta \to \infty$, the only way for the integral in Equation (3.25) to diverge to give an infinite or very large β is for the denominator to vanish. This only occurs for $V(\bar{z}) \to 0$ and for $c \to 0$. $V(\bar{z}) \to 0$ occurs as $\bar{z} \to \pm a$, which is near the start and end of the trajectory. Also, physically, if the particle is to interpolate from $-a$ to a in a longer and longer time, β, then it must start out at $-a$ with a smaller and smaller initial velocity, c. For larger and larger β, c must vanish in an appropriate fashion. Heuristically, for small c, the solution spends most of its time near $\bar{z} = \pm a$ and interpolates from one to the other relatively quickly. Then the major contribution to the integral comes from the region around $\bar{z} = \pm a$. Since the integral diverges logarithmically when $c = 0$, for a typical potential V (which must vanish quadratically at $\bar{z} = \pm a$ as V has a double zero at $\pm a$), the integral must behave as $-\ln c$, *i.e.* $\beta \sim -\ln c$ which is equivalent to $c \sim e^{-\beta}$, which means that c must vanish exponentially with large β. For sufficiently large β we may neglect c altogether.

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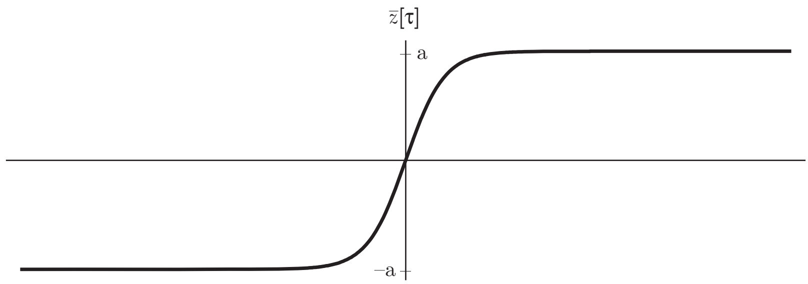

Figure 3.3. Interpolating kink instanton for the symmetric double well

The action for the constant solutions, Equation (3.21), is evidently zero. For the interpolating solution implicitly determined by Equation (3.24), it is

$$\begin{aligned} S_E[\bar{z}(\tau)] &= \int_{-\frac{\beta}{2}}^{\frac{\beta}{2}} d\tau \left(\frac{1}{2}\dot{\bar{z}}^2(\tau) + V(\bar{z}(\tau))\right) \\ &= \int_{-\frac{\beta}{2}}^{\frac{\beta}{2}} d\tau \left(\dot{\bar{z}}^2(\tau) - c^2\right) \\ &= \left(\int_{-\frac{\beta}{2}}^{\frac{\beta}{2}} \sqrt{2V(\bar{z}(\tau)) + c^2}\,\frac{d\bar{z}}{d\tau} d\tau\right) - \beta c^2 \\ &= \left(\int_{-a}^{a} d\bar{z}\sqrt{2V(\bar{z}) + c^2}\right) - \beta c^2. \end{aligned} \tag{3.26}$$

For large β, we neglect c in the integral for $S_E[\bar{z}(\tau)] \equiv S_0$, and the term $-\beta c^2$, yielding

$$S_0 = \int_{-a}^{a} d\bar{z}\sqrt{2V(\bar{z})}. \tag{3.27}$$

This is exactly the action corresponding to the classical solution for $\beta = \infty$ depicted in Figure 3.3. Such Euclidean time classical solutions are called "instantons".

For large τ the approximate equation satisfied by $\bar{z}(\tau)$ is

$$\frac{d\bar{z}}{d\tau} = \omega(a - \bar{z}), \tag{3.28}$$

obtained by expanding Equation (3.23) as $\bar{z} \to a^-$ from below and where ω^2 is the second derivative of the potential at $\bar{z} = a$. There is a corresponding, equivalent analysis for $\tau \to -\infty$. These have the solution

$$|z(\tau)| = a - Ce^{-\omega|\tau|}. \tag{3.29}$$

Thus the instanton is exponentially close to $\pm a$ for $|\tau| > \frac{1}{\omega}$. Its size is $\frac{1}{\omega}$ which is of order 1, compared with $\hbar$ and β. For large $|\tau|$, the solution is essentially equal to $\pm a$, which is just the trivial solution. The solution is "on" only for an

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"instant", the relatively short time compared with β, during which it interpolates between $-a$ and $+a$. Hence the name instanton. Reversing the time direction gives another solution which starts at $+a$ and interpolates to $-a$, aptly called an anti-instanton. It clearly has the same action as an instanton.

3.4 The Instanton Contribution to the Path Integral

3.4.1 Translational Invariance Zero Mode

As we have seen, for very large β, the instanton corresponding to infinite β is an arbitrarily close and perfectly good approximation to the true instanton. Evidently with the infinite β instanton, we may choose the time arbitrarily at which the solution crosses over from $-a$ to $+a$. The solution of

$$\int_0^{\bar{z}(\tau)} \frac{dz}{\sqrt{2V(z)}} = \tau - \tau_0 \tag{3.30}$$

corresponds to an instanton which crosses over around $\tau = \tau_0$. Thus the position of the instanton τ_0 gives a one-parameter family of solutions, each with the same classical action. The point is that for large enough β, there exists a one-parameter family of approximate critical points with action arbitrarily close to S_0. The contribution to the path integral from the vicinity of these approximate critical points will be of a slightly modified form, since the first variation of the action about the approximate critical point does not quite vanish. Thus the contribution will be of the form, the exponential of the negative action at the approximate critical point, multiplied by a Gaussian integral with a linear shift, the shift coming from the non-vanishing first variation of the action. The shift will be proportional to some arbitrarily small function $f(\beta)$ as $\beta \to \infty$. The higher-order terms give perturbative corrections in $\hbar$, as in Equation (3.16), and can be dropped. Then, considering a typical Gaussian integral with a small linear shift, as arises in the integration about an approximate critical point, we have

$$\int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi}} e^{-\frac{1}{\hbar}\left(\alpha^2 x^2 + 2f(\beta)x\right)} = e^{\frac{f^2(\beta)}{\hbar\alpha^2}} \frac{1}{\alpha}. \tag{3.31}$$

We see that to be able to neglect the effects of the shift, $f(\beta)$ must be so small that $\frac{f^2(\beta)}{\hbar} \ll 1$, given that α, being independent of $\hbar$ and β, is of order 1.

Typically, $f(\beta)$ is exponentially small in β, just as earlier c was found to be. $f(\beta)$ needs to be determined and depends of the details of the dynamics. In any case, β must be greater than a certain value determined by the value of $\hbar$. This is, however, no strong constraint other than imposing that we must consider the limit that β is arbitrarily large while all other constants (especially $\hbar$) are held fixed. Hence, assuming β is sufficiently large, we can neglect the effect of the linear shift and we must include the contribution from these approximate critical points. To do so, we simply integrate over the position of the instanton and perform the Gaussian integral over directions in path space which are orthogonal to the direction corresponding to translations of the instanton.

The easiest way to perform such a constrained Gaussian integral is to use the following observations. In the infinite β limit, the translated instantons become exact critical points and correspondingly the fluctuation directions about a given instanton contain a flat direction. This means that the action does not change to second order for variations along this direction. Precisely, this means that the eigenfrequencies, λ_n, contain a zero mode, $\lambda_0 = 0$. We can explicitly construct this zero mode since

$$\left(-\frac{d^2}{d\tau^2} + V''(\bar{z}(\tau-\tau_1))\right)\frac{d\bar{z}(\tau-\tau_1)}{d\tau_1} = -\frac{d}{d\tau}\left(-\ddot{\bar{z}}(\tau-\tau_1) + V'(\bar{z}(\tau-\tau_1))\right) = 0, \tag{3.32}$$

the second term vanishing by the equation of motion, Equation (3.20), which is clearly also valid for $\bar{z}(\tau-\tau_1)$. This mode occurs because of the time translation invariance when β is infinite. The corresponding normalized zero mode is

$$z_0(\tau) = \frac{1}{\sqrt{S_0}}\frac{d}{d\tau_1}\bar{z}(\tau-\tau_1). \tag{3.33}$$

Clearly

$$\int_{-\infty}^{\infty} d\tau \left(\frac{1}{\sqrt{S_0}}\frac{d}{d\tau_1}\bar{z}(\tau-\tau_1)\right)^2 = \frac{1}{S_0}\int_{-\infty}^{\infty} d\tau \left(\frac{1}{2}\dot{\bar{z}}^2(\tau-\tau_1) + V(\bar{z}(\tau-\tau_1))\right) = 1 \tag{3.34}$$

using the equation of motion, Equation (3.23), with $c = 0$ (infinite β).

Integration in the path integral, Equation (3.15), over the coefficient of this mode yields a divergence as the frequency is zero

$$\int \frac{dc_0}{\sqrt{2\pi\hbar}} e^{-\frac{1}{\hbar}\lambda_0 c_0^2} = \int \frac{dc_0}{\sqrt{2\pi\hbar}} 1 = \infty. \tag{3.35}$$

However, integrating over the position of the instanton is equivalent to integrating over c_0. τ_1 is called a collective coordinate of the instanton corresponding to its position in Euclidean time. Indeed, if $\bar{z}(\tau-\tau_1)$ is an instanton at position τ_1, the change in the path obtained by infinitesimally changing τ_1 is

$$\delta z(\tau) = \frac{d}{d\tau_1}\bar{z}(\tau-\tau_1)d\tau_1 = \sqrt{S_0}z_0(\tau). \tag{3.36}$$

The change induced by varying c_0 is, however,

$$\delta z(\tau) = z_0(\tau)dc_0. \tag{3.37}$$

Thus

$$\frac{dc_0}{\sqrt{2\pi\hbar}} = \sqrt{\frac{S_0}{2\pi\hbar}}d\tau_1 \tag{3.38}$$

and when integrating over the position τ_1 we should multiply by the normalizing factor $\sqrt{\frac{S_0}{2\pi\hbar}}$. Clearly for infinite β the integral over τ_1 diverges, reflecting the equivalent infinity obtained when integrating over c_0.

This divergence is not disturbing, since for a positive definite Hamiltonian the infinite β limit of the matrix element, Equation (2.32), is strictly zero, and for large β it is an expression which vanishes exponentially. Thus in the large β limit, the Gaussian integrals in the directions orthogonal to the flat direction must combine to give an expression which indeed vanishes exponentially with β, as we will see. For the time being, for finite β, the integration over the position then gives a factor that is linear in β

$$\sqrt{\frac{S_0}{2\pi\hbar}}\beta. \tag{3.39}$$

Thus, so far the path integral has yielded

$$\langle a|e^{-\frac{\beta}{\hbar}\hat{h}(\hat{X},\hat{P})}|-a\rangle = e^{-\frac{S_0}{\hbar}}\left(\frac{S_0}{2\pi\hbar}\right)^{\frac{1}{2}}\beta\mathcal{N}\left(\det{}'\left[-\frac{d^2}{d\tau^2}+V''(\bar{z}(\tau)\right]\right)^{-\frac{1}{2}}, \tag{3.40}$$

where $\det'$ means the "determinant" excluding the zero eigenvalue. We will leave the evaluation of the determinant for a little later when will show that

$$\mathcal{N}\left(\det{}'\left[-\frac{d^2}{d\tau^2}+V''(\bar{z}(\tau))\right]\right)^{-\frac{1}{2}} = K\mathcal{N}\left(\det\left[-\frac{d^2}{d\tau^2}+\omega^2\right]\right)^{-\frac{1}{2}}, \tag{3.41}$$

where ω was defined at Equation (3.28), and we will evaluate K, which is, most importantly, independent of $\hbar$ and β.

3.4.2 Multi-instanton Contribution

To proceed further, we must realize that there are also other approximate critical points which give significant contributions to the path integral. These correspond to classical configurations which have, for example, an instanton at τ_1, an anti-instanton at τ_2 and again an instanton at τ_3. If τ_i are well separated within the interval β, these configurations are approximately critical, with an error of the same order as for the approximate critical points previously considered. More generally we can have a string of n pairs of an instanton followed by an anti-instanton, plus a final instanton completing the interpolation from $-a$ to a. We denote such a configuration as $\bar{z}_{2n+1}(\tau)$. The positions are arbitrary except that the order of the instantons and the anti-instantons must be preserved and they must be well separated. The action for $2n+1$ such objects is just $(2n+1)S_0$ to the same degree of accuracy.

One would, at first sight, conclude that this contribution, including the Gaussian integral about these approximate critical points, is exponentially suppressed relative to the contribution from the single instanton sector. Indeed, we would find that the contribution of the $2n+1$-instantons and anti-instantons

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to the matrix element[1],

$$\langle a|e^{-\frac{\beta}{\hbar}\hat{h}(\hat{X},\hat{P})}|-a\rangle_{2n+1}=e^{-\frac{(2n+1)S_0}{\hbar}}\mathcal{N}\left(\det\left[-\frac{d^2}{d\tau^2}+V''(\bar{z}_{2n+1}(\tau)\right]\right)^{-\frac{1}{2}} \tag{3.42}$$

is suppressed by $e^{-\frac{2nS_0}{\hbar}}$ relative to the one instanton contribution. This is true; however, we must analyse the effects of zero modes.

For $2n+1$ instantons and anti-instantons there are $2n+1$ zero modes corresponding to the independent translation of each object. This is actually only true for infinitely separated objects with β infinite; however, for β large, it is an arbitrarily good approximation. Thus there exist $2n+1$ zero frequencies in the determinant which should not be included in the path integration and, correspondingly, we should integrate over the positions of the $2n+1$ instantons and anti-instantons. This integration is constrained by the condition that their order is preserved. Hence we get the factor

$$\int_{-\frac{\beta}{2}}^{\frac{\beta}{2}}d\tau_1\int_{\tau_1}^{\frac{\beta}{2}}d\tau_2\int_{\tau_2}^{\frac{\beta}{2}}d\tau_3\cdots\int_{\tau_{2n-1}}^{\frac{\beta}{2}}d\tau_{2n}\int_{\tau_{2n}}^{\frac{\beta}{2}}d\tau_{2n+1}=\frac{\beta^{2n+1}}{(2n+1)!}. \tag{3.43}$$

Furthermore, from exactly the same analysis as the integration over the position of the single instanton, the integration is normalized correctly only when each factor is multiplied by $\left(\frac{S_0}{2\pi\hbar}\right)^{\frac{1}{2}}$. Thus we find

$$\begin{aligned}&\left\langle a\left|e^{-\frac{\beta}{\hbar}\hat{h}(\hat{X},\hat{P})}\right|-a\right\rangle_{2n+1}\\&=\left(e^{-\frac{S_0}{\hbar}}\left(\frac{S_0}{2\pi\hbar}\right)^{\frac{1}{2}}\beta\right)^{2n+1}\frac{\mathcal{N}}{(2n+1)!}\left(\det{}'\left[-\frac{d^2}{d\tau^2}+V''(\bar{z}_{2n+1}(\tau))\right]\right)^{-\frac{1}{2}},\end{aligned} \tag{3.44}$$

where $\det'$ again means the determinant with the $2n+1$ zero modes removed. We will show later that

$$\mathcal{N}\left(\det{}'\left[-\frac{d^2}{d\tau^2}+V''(\bar{z}_{2n+1}(\tau))\right]\right)^{-\frac{1}{2}}=K^{2n+1}\mathcal{N}\left(\det\left[-\frac{d^2}{d\tau^2}+\omega^2\right]\right)^{-\frac{1}{2}} \tag{3.45}$$

for the same K as in the case of one instanton, as in Equation (3.41).

Now even if $e^{-\frac{S_0}{\hbar}}$ is very small, our whole analysis is done at fixed $\hbar$ with $\beta\to\infty$; the relevant parameter, as can be seen from Equation (3.44), is

$$\delta=\left(\frac{S_0}{2\pi\hbar}\right)^{\frac{1}{2}}e^{-\frac{S_0}{\hbar}}K\beta, \tag{3.46}$$

which is arbitrarily large in this limit. Thus it seems that the contribution from the strings of instanton and anti-instanton pairs is proportional to δ^{2n+1} and

[1] Here the subscript $2n+1$ signifies that we are calculating only the contribution to the matrix element from $2n+1$ instantons and anti-instantons.

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seems to get larger and larger. However, the denominator contains $(2n+1)!$, which must be taken into account. For large enough n, the denominator always dominates, $\delta^{2n+1} \ll (2n+1)!$, and so renders the contribution small.

We require, however, for the consistency of our approximations that when n is large enough so that this is true, the average space per instanton or anti-instanton, $\frac{\beta}{2n+1}$, is still large compared to the size of these objects $\sim 1/\omega$, which is independent of both $\hbar$ and β. This is satisfied as $\beta \to \infty$. Hence we require n large enough such that

$$\frac{\delta^{2n+1}}{(2n+1)!} \ll 1; \tag{3.47}$$

however, with

$$\frac{\beta}{2n+1} \gg \frac{1}{\omega}. \tag{3.48}$$

Taking the logarithm of Equation (3.47) after multiplying by $(2n+1)!$ yields in the Stirling approximation

$$(2n+1)\ln\delta \ll (2n+1)\ln(2n+1) - (2n+1). \tag{3.49}$$

Neglecting the second term on the right-hand side and combining with Equation (3.48) yields

$$\delta = \left(\left(\frac{S_0}{2\pi\hbar}\right)^{\frac{1}{2}} e^{-\frac{S_0}{\hbar}} K\right)\beta \ll 2n+1 \ll \omega\beta. \tag{3.50}$$

That such an n can exist simply requires $\left(\frac{S_0}{2\pi\hbar}\right)^{\frac{1}{2}} e^{-\frac{S_0}{\hbar}} K \lll \omega$. We will evaluate K explicitly and find that it does not depend on $\hbar$ or β. The inequality then is clearly satisfied for $\hbar \to 0$, which brings into focus that underneath everything we are interested in the semi-classical limit.

A tiny parenthetical remark is in order: in integrating over the positions of the instantons, we should always maintain the constraint that the instantons are well separated. Thus we should not integrate the position of one instanton exactly from that of the preceding one to that of the succeeding one, but we should leave a gap of the order of $\frac{1}{\omega}$ which is the size of the instanton. Such a correction corresponds to a contribution which behaves to leading order as $\frac{1}{\omega}\frac{\beta^{n-1}}{(n-1)!}$, which is negligible in comparison to $\frac{\beta^n}{n!}$ if $\frac{1}{\omega} \ll \beta$.

When the density of instantons and anti-instantons becomes large, all of our approximations break down, and such configurations are no longer even approximately critical. Thus we do not expect any significant contribution to the path integral from the regions of the space of paths which include these configurations. Hence we should actually truncate the series in the number of instantons for some large enough n; however, this is not necessary. We will always assume that we work in the limit that β should be sufficiently large and $\hbar$ sufficiently small so that the contribution from the terms in the series with

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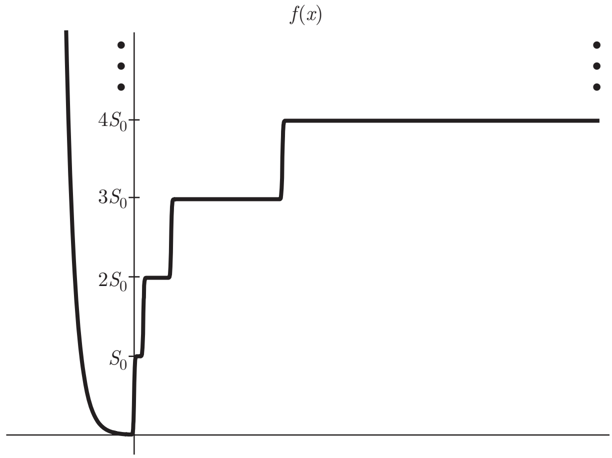

Figure 3.4. A simple function analogous to the action

n greater than some N is already negligible, while there is still a lot of room per instanton, *i.e.* β/N is still large. This should still correspond to a dilute "gas" of instantons and anti-instantons. Then the remaining terms in the series can be maintained, although they do not represent the contribution from any part of path space. It is simply easier to sum the series to infinity, knowing that the contribution added in from n greater than some N makes only a negligible change. The sum to infinity is straightforward. We find

$$\left\langle a \left| e^{-\frac{\beta}{\hbar}\hat{h}(\hat{X},\hat{P})} \right| -a \right\rangle = \left(\mathcal{N} \left(\det \left[-\frac{d^2}{d\tau^2} + \omega^2 \right] \right)^{-\frac{1}{2}} \right) \sinh \left(\left(\frac{S_0}{2\pi\hbar} \right)^{\frac{1}{2}} e^{-\frac{S_0}{\hbar}} K\beta \right). \tag{3.51}$$

3.4.3 Two-dimensional Integral Paradigm

A simple two-dimensional, ordinary integral which serves as a paradigm exhibiting many of the features of the path integral just considered is given by

$$\mathcal{I} = \int dxdy e^{-\frac{1}{\hbar}(f(x)+\frac{\alpha^2}{2}y^2)} \tag{3.52}$$

where y corresponds to the transverse directions and plays no role. $f(x)$ is a function of the form depicted in Figure 3.4 and increases sharply in steps of S_0, and the length of each plateau is $\frac{\beta^n}{n!}$. In the limit that the steps become sharp, the integral can be done exactly and yields

$$\mathcal{I} = \frac{(2\pi\hbar)^{\frac{1}{2}}}{\alpha} \sum_{n=0}^{\infty} e^{-\frac{nS_0}{\hbar}} \left(\frac{\beta^n}{n!} \right) = \frac{(2\pi\hbar)^{\frac{1}{2}}}{\alpha} e^{\left(\beta e^{-\frac{S_0}{\hbar}}\right)}. \tag{3.53}$$

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Obviously this is exactly analogous to the path integral just considered for $\beta \to \infty$ and $\hbar \to 0$. The plateaux correspond to the critical points. Clearly we cannot consider just the lowest critical point since the volume associated with the higher critical points is sufficiently large that their contribution does not damp out until n becomes large enough. In terms of physically intuitive arguments, the volume is like the entropy factor associated with n instantons, $\frac{\beta^n}{n!}$, while the exponential, $e^{-\frac{nS_0}{\hbar}}$, is like the Boltzmann factor. In statistical mechanics, even though the Boltzmann factor is much smaller for higher energy levels, their contribution to the partition function can be significant due to a large enough entropy. We can further model the aspect of approximate critical points by giving the plateaux in Figure 3.4 a very small slope. Clearly the integral is only negligibly modified if the slope is taken to be exponentially small in β.

3.5 Evaluation of the Determinant

Finally, we are left with the evaluation of the determinant. We wish to show for the case of $2n+1$ instantons and anti-instantons

$$\left(\mathcal{N}\left(\det{}'\left[-\frac{d^2}{d\tau^2}+V''(\bar{z}_{2n+1}(\tau))\right]\right)^{-\frac{1}{2}}\right)=K^{2n+1}\left(\mathcal{N}\left(\det\left[-\frac{d^2}{d\tau^2}+\omega^2\right]\right)^{-\frac{1}{2}}\right) \tag{3.54}$$

and to evaluate K. Physically this means that the effect of each instanton and anti-instanton is simply to multiply the free determinant by a factor of $\frac{1}{K^2}$. Intuitively this is very reasonable, and we expect that for well-separated instantons their effect would be independent of each other.

To obtain the $\det'$ we will work in the finite large interval, β, with boundary conditions that the wave function must vanish at the end points. Consider first the case of just one instanton. Because of the finite interval, time translation will not be an exact symmetry and the operator $-\frac{d^2}{d\tau^2}+V''(\bar{z}(\tau))$ will not have an exact zero mode. However, as $\beta \to \infty$ one mode will approach zero. The $\det'$ is then obtained by calculating the full determinant on the finite interval, β, and then dividing out by the smallest eigenvalue. There should be a rigorous theorem proving first that the operator in question has a positive definite spectrum on the finite interval, β, for any potential, $V(z)$, of the type considered and the corresponding instanton, $\bar{z}(\tau)$, and secondly as $\beta \to \infty$, one bound state drops to exactly zero; this is reasonable and taken as a hypothesis. Thus we will study the full determinant on the interval β which has the path-integral representation

$$\begin{aligned}&\mathcal{N}\left(\det\left[-\frac{d^2}{d\tau^2}+V''(\bar{z}(\tau-\tau_1))\right]\right)^{-\frac{1}{2}}\\ &\quad=\mathcal{N}\int \mathcal{D}z(\tau)e^{-\frac{1}{\hbar}\int_{-\frac{\beta}{2}}^{\frac{\beta}{2}}d\tau\frac{1}{2}\left(\dot{z}^2(\tau)+V''(\bar{z}(\tau-\tau_1))z^2(\tau)\right)}\end{aligned} \tag{3.55}$$

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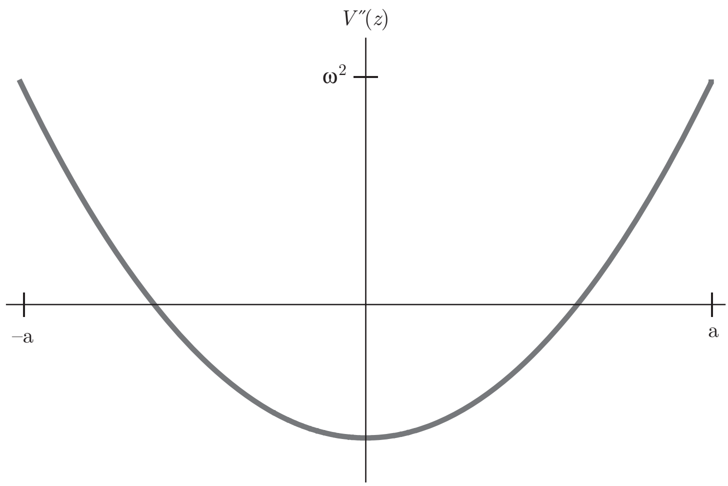

Figure 3.5. The behaviour of $V''(z)$ between $\pm a$

with the boundary conditions that $z(\frac{\beta}{2}) = z(-\frac{\beta}{2}) = 0$ in the path integral. The path integral on the right-hand side is performed in exactly the same manner as in Equation (3.15). This determinant actually corresponds to the matrix element of the Euclidean time evolution operator with a time-dependent Hamiltonian,

$$\langle z=0|\mathcal{T}\left(e^{-\frac{1}{\hbar}\int_{-\frac{\beta}{2}}^{\frac{\beta}{2}} d\tau\left(\frac{1}{2}\hat{P}^2+\frac{V''(\bar{z}(\tau-\tau_1))}{2}\hat{X}^2\right)}\right)|z=0\rangle, \tag{3.56}$$

where $\mathcal{T}$ denotes the operation of Euclidean time ordering. This time ordering is effectively described by the product representation of Equation (2.33), where the appropriate Hamiltonian is entered into each Euclidean time slice. This can be shown to give the path integral, Equation (3.55), adapting with minimal changes the demonstration in Chapter 2. We leave it to the reader to confirm the details.

Consider first the behaviour of $V''(z)$ which controls the Euclidean time-dependent frequency in the path integral Equation (3.55). $V''(\pm a) = \omega^2$ is the parabolic curvature at the bottom of each well. In between, at $z = 0$, $V''(0)$ will drop to some negative value giving the curvature at the top of the potential hill separating the two wells. We will have a function as depicted in Figure 3.5. Thus $V''(\bar{z}(\tau))$ will start out at ω^2 at $\tau = -\infty$, until $\bar{z}(\tau)$ starts to cross over from $-a$ to a, where it will trace out the potential well of Figure 3.5, and again it will regain the value ω^2 for $\bar{z}(\tau) = a$ at $\tau = \infty$, corresponding to the function of τ as in Figure 3.6. Thus the path integral in Equation (3.55) is exactly equal to the matrix element or "Euclidean persistence amplitude" that a particle at position zero will remain at position zero in Euclidean time β in a quadratic potential with a time-dependent frequency given by $V''(\bar{z}(\tau))$ depicted in Figure 3.6.

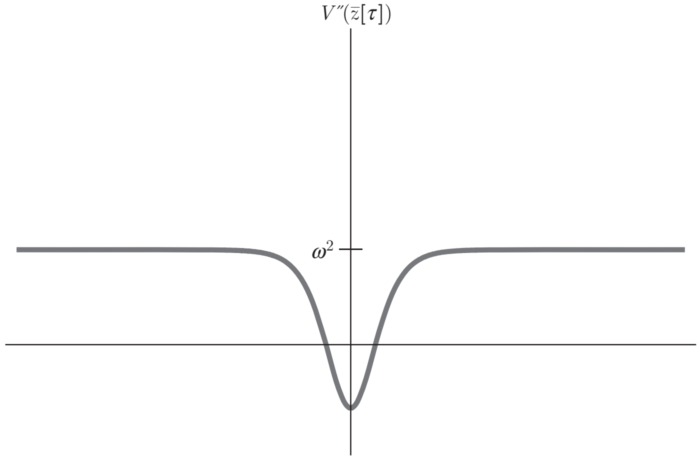

Figure 3.6. The behaviour of $V''(z(\tau)$ between $\tau=\pm\infty$

We will express the matrix element in terms of a Euclidean time evolution operator $\mathcal{U}\left(\frac{\beta}{2},-\frac{\beta}{2}\right)$ as

$$\mathcal{N}\int\mathcal{D}z(\tau)e^{-\frac{1}{\hbar}\int_{-\frac{\beta}{2}}^{\frac{\beta}{2}}d\tau\frac{1}{2}\left(\dot{z}^2(\tau)+V''(\bar{z}(\tau-\tau_1))z^2(\tau)\right)}\equiv\left\langle z=0\left|\mathcal{U}\left(\tfrac{\beta}{2},-\tfrac{\beta}{2}\right)\right|z=0\right\rangle \quad (3.57)$$

with explicitly,

$$\mathcal{U}\left(\tfrac{\beta}{2},-\tfrac{\beta}{2}\right)=\mathcal{T}\left(e^{-\frac{1}{\hbar}\int_{-\frac{\beta}{2}}^{\frac{\beta}{2}}d\tau\left(\frac{1}{2}\hat{P}^2+\frac{V''(\bar{z}(\tau-\tau_1))}{2}\hat{X}^2\right)}\right). \quad (3.58)$$

Now

$$\begin{aligned}\mathcal{U}\left(\tfrac{\beta}{2},-\tfrac{\beta}{2}\right)&=\mathcal{U}\left(\tfrac{\beta}{2},\tau_1+\tfrac{1}{2\omega}\right)\mathcal{U}\left(\tau_1+\tfrac{1}{2\omega},\tau_1-\tfrac{1}{2\omega}\right)\mathcal{U}\left(\tau_1-\tfrac{1}{2\omega},-\tfrac{\beta}{2}\right)\\&\approx\mathcal{U}^0\left(\tfrac{\beta}{2},\tau_1+\tfrac{1}{2\omega}\right)\mathcal{U}\left(\tau_1+\tfrac{1}{2\omega},\tau_1-\tfrac{1}{2\omega}\right)\mathcal{U}^0\left(\tau_1-\tfrac{1}{2\omega},-\tfrac{\beta}{2}\right),\end{aligned} \quad (3.59)$$

where on the intervals $\left[\tau_1+\frac{1}{2\omega},\frac{\beta}{2}\right]$ and $\left[-\frac{\beta}{2},\tau_1-\frac{1}{2\omega}\right]$ we can replace the full evolution operator with the free evolution operator

$$\mathcal{U}^0(\tau,\tau')=T\left(e^{-\frac{1}{\hbar}\int_{\tau'}^{\tau}d\tau\frac{1}{2}\left(-\hbar^2\frac{d^2}{dz^2}+\omega^2z^2\right)}\right)=e^{-\frac{(\tau-\tau')}{\hbar}\hat{h}^0(\hat{X},\hat{P})} \quad (3.60)$$

as $V''(\bar{z}(\tau)$ is essentially constant and equal to ω^2 on these intervals. Then inserting complete sets of free eigenstates, which are just simple harmonic oscillator states $|E_n\rangle$ for an oscillator of frequency ω , we obtain

$$\begin{aligned}\mathcal{U}\left(\tfrac{\beta}{2},-\tfrac{\beta}{2}\right)=\sum_{n,m}&e^{-\left(\frac{\beta}{2}-\tau_1-\frac{1}{2\omega}\right)\frac{E_n}{\hbar}}|E_n\rangle\langle E_n|\mathcal{U}\left(\tau_1+\tfrac{1}{2\omega},\tau_1-\tfrac{1}{2\omega}\right)|E_m\rangle\\&\times\langle E_m|\,e^{-\left(\tau_1-\frac{1}{2\omega}+\frac{\beta}{2}\right)\frac{E_m}{\hbar}}\end{aligned} \quad (3.61)$$

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Now we use the "ground state saturation approximation", *i.e.* when β is huge and the instanton is not near the boundaries, only the ground state contribution is important. Using this twice we obtain

$$\begin{aligned}
\mathcal{U}\left(\tfrac{\beta}{2},-\tfrac{\beta}{2}\right) &\approx e^{\left(\frac{\beta}{2}-\tau_1-\frac{1}{2\omega}\right)\frac{E_0}{\hbar}}\left|E_0\right\rangle\left\langle E_0\right|\mathcal{U}\left(\tau_1+\tfrac{1}{2\omega},\tau_1-\tfrac{1}{2\omega}\right)\left|E_0\right\rangle\left\langle E_0\right|e^{-\left(\tau_1-\frac{1}{2\omega}+\frac{\beta}{2}\right)\frac{E_0}{\hbar}}\\
&=\mathcal{U}^0\left(\tfrac{\beta}{2},\tau_1+\tfrac{1}{2\omega}\right)\left|E_0\right\rangle\left\langle E_0\right|\mathcal{U}^0\left(\tau_1+\tfrac{1}{2\omega},\tau_1-\tfrac{1}{2\omega}\right)\left|E_0\right\rangle\left\langle E_0\right|\mathcal{U}^0\left(\tau_1-\tfrac{1}{2\omega},-\tfrac{\beta}{2}\right)\times\\
&\quad\times\frac{\left\langle E_0\right|\mathcal{U}\left(\tau_1+\frac{1}{2\omega},\tau_1-\frac{1}{2\omega}\right)\left|E_0\right\rangle}{\left\langle E_0\right|\mathcal{U}^0\left(\tau_1+\frac{1}{2\omega},\tau_1-\frac{1}{2\omega}\right)\left|E_0\right\rangle}\\
&\approx\sum_{n,m}\mathcal{U}^0\left(\tfrac{\beta}{2},\tau_1+\tfrac{1}{2\omega}\right)\left|E_n\right\rangle\left\langle E_n\right|\mathcal{U}^0\left(\tau_1+\tfrac{1}{2\omega},\tau_1-\tfrac{1}{2\omega}\right)\left|E_m\right\rangle\left\langle E_m\right|\mathcal{U}^0\left(\tau_1-\tfrac{1}{2\omega},-\tfrac{\beta}{2}\right)\times\\
&\quad\times\frac{\left\langle E_0\right|\mathcal{U}\left(\tau_1+\frac{1}{2\omega},\tau_1-\frac{1}{2\omega}\right)\left|E_0\right\rangle}{\left\langle E_0\right|\mathcal{U}^0\left(\tau_1+\frac{1}{2\omega},\tau_1-\frac{1}{2\omega}\right)\left|E_0\right\rangle}\\
&=\mathcal{U}^0\left(\tfrac{\beta}{2},-\tfrac{\beta}{2}\right)\frac{\left\langle E_0\right|\mathcal{U}\left(\tau_1+\frac{1}{2\omega},\tau_1-\frac{1}{2\omega}\right)\left|E_0\right\rangle}{\left\langle E_0\right|\mathcal{U}^0\left(\tau_1+\frac{1}{2\omega},\tau_1-\frac{1}{2\omega}\right)\left|E_0\right\rangle}\\
&\equiv\mathcal{U}^0\left(\tfrac{\beta}{2},-\tfrac{\beta}{2}\right)\kappa, \qquad (3.62)
\end{aligned}$$

where κ is the ratio of the two amplitudes over the short time period during which $V''(\bar{z}(\tau)$ is non-trivially time-dependent. κ is surely independent of the position τ_1 of the instanton. The full evolution operator in fact simply does not depend on the position, nor does the denominator. Indeed,

$$\begin{aligned}
\mathcal{U}\left(\tau_1+\tfrac{1}{2\omega},\tau_1-\tfrac{1}{2\omega}\right) &= T\left(e^{-\frac{1}{\hbar}\int_{\tau_1-\frac{1}{2\omega}}^{\tau_1+\frac{1}{2\omega}}d\tau\,\frac{1}{2}\left(-\hbar^2\frac{d^2}{dz^2}+V''(\bar{z}(\tau-\tau_1))z^2\right)}\right)\\
&= T\left(e^{-\frac{1}{\hbar}\int_{-\frac{1}{2\omega}}^{\frac{1}{2\omega}}d\tau'\,\frac{1}{2}\left(-\hbar^2\frac{d^2}{dz^2}+V''(\bar{z}(\tau'))z^2\right)}\right), \qquad (3.63)
\end{aligned}$$

since the integration variable is a dummy, thus exhibiting manifest τ_1 independence.

Clearly for n well-separated instantons the result applies also, we simply apply an appropriately adapted version of the same arguments. We convert the determinant into a persistence amplitude for the related quadratic quantum mechanical process, which we then further break up into free evolution in the gaps between the instantons and full evolution during the instanton, use the ground state saturation approximation, giving the result, to leading approximation

$$\mathcal{N}\left(\det\left[-\frac{d^2}{d\tau^2}+V''(\bar{z}_{2n+1}(\tau))\right]\right)^{-\frac{1}{2}}=\mathcal{N}\left(\det\left[-\frac{d^2}{d\tau^2}+\omega^2\right]\right)^{-\frac{1}{2}}\kappa^{2n+1}. \quad (3.64)$$

The relationship of κ to the K fixed by Equation (3.41) is obtained by dividing out by the lowest energy eigenvalue, call it λ_0. We will show that this eigenvalue is exponentially small for large β. For $2n+1$ instantons there are $2n+1$ such eigenvalues which are all equal, in first approximation, and we must remove them all giving

$$\mathcal{N}\left(\det'\left[-\frac{d^2}{d\tau^2}+V''(\bar{z}_{2n+1}(\tau))\right]\right)^{-\frac{1}{2}} = \mathcal{N}\left(\frac{\det\left[-\frac{d^2}{d\tau^2}+V''(\bar{z}_{2n+1}(\tau))\right]}{\lambda_0^{2n+1}}\right)^{-\frac{1}{2}}$$
$$= \mathcal{N}\left(\det\left[-\frac{d^2}{d\tau^2}+\omega^2\right]\right)^{-\frac{1}{2}}\left(\kappa\lambda_0^{\frac{1}{2}}\right)^{2n+1} \quad (3.65)$$

Hence

$$K = \kappa\lambda_0^{\frac{1}{2}}. \quad (3.66)$$

It only remains to calculate two things, the free determinant and the correction factor K.

3.5.1 Calculation of the Free Determinant

To calculate the free determinant, we will use the method of Affleck and Coleman [31, 114, 36]. Consider the more general case

$$\det\left[-\frac{d^2}{d\tau^2}+W(\tau)\right], \quad (3.67)$$

where the operator acts on the space of functions which vanish at $\pm\frac{\beta}{2}$. Formally we want to compute the infinite product of the eigenvalues of the eigenvalue problem

$$\left(-\frac{d^2}{d\tau^2}+W(\tau)\right)\psi_{\lambda_n}(\tau) = \lambda_n\psi_{\lambda_n}(\tau), \quad \psi_{\lambda_n}\left(\pm\frac{\beta}{2}\right) = 0. \quad (3.68)$$

The eigenvalues generally increase unboundedly, hence the infinite product is actually ill-defined. Consider, nevertheless, an ancillary problem

$$\left(-\frac{d^2}{d\tau^2}+W(\tau)\right)\psi_\lambda(\tau) = \lambda\psi_\lambda(\tau), \quad \psi_\lambda\left(-\frac{\beta}{2}\right) = 0, \quad \left.\frac{d}{d\tau}\psi_\lambda(\tau)\right|_{-\frac{\beta}{2}} = 1. \quad (3.69)$$

There exists, in general, a solution for each λ; the second boundary condition can always be satisfied by adjusting the normalization. On the other hand, the equation in λ

$$\psi_\lambda\left(\frac{\beta}{2}\right) = 0 \quad (3.70)$$

has solutions exactly at the eigenvalues $\lambda = \lambda_n$. Affleck and Coleman [31, 114, 36] propose to define the ratio of the determinant for two different potentials as

$$\frac{\det\left[-\frac{d^2}{d\tau^2}+W_1(\tau)-\lambda\right]}{\det\left[-\frac{d^2}{d\tau^2}+W_2(\tau)-\lambda\right]} = \frac{\psi_\lambda^1\left(\frac{\beta}{2}\right)}{\psi_\lambda^2\left(\frac{\beta}{2}\right)}. \quad (3.71)$$

The left-hand side is defined as the infinite product

$$\prod_{n=1}^{\infty} \frac{(\lambda_n^1 - \lambda)}{(\lambda_n^2 - \lambda)}, \tag{3.72}$$

where the potentials and the labelling of the eigenvalues are assumed to be such that as the eigenvalues become large, they approach each other sufficiently fast,

$$\lim_{n\to\infty} (\lambda_n^1 - \lambda_n^2) = 0 \tag{3.73}$$

so that the infinite product in Equation (3.72) does conceivably converge. To prove Equation (3.71) we observe that the zeros, $\lambda = \lambda_n^1$, and poles, $\lambda = \lambda_n^2$, of the left-hand side are at the same place as those of the right-hand side, as evinced by the solutions of Equation (3.70). Thus the ratio of the two sides

$$\frac{\prod_{n=1}^{\infty} \frac{(\lambda_n^1-\lambda)}{(\lambda_n^2-\lambda)}}{\psi_\lambda^1\left(\frac{\beta}{2}\right) / \psi_\lambda^2\left(\frac{\beta}{2}\right)} \equiv g(\lambda) \tag{3.74}$$

defines an analytic function $g(\lambda)$ without zeros or poles. Now as $|\lambda| \to \infty$ in all directions except the real axis, the numerator in Equation (3.74) is equal to 1. For the denominator, as $\lambda \to \infty$ the potentials W_1 and W_2 become negligible perturbations compared to the term on the right-hand side of Equation (3.69), which we can consider as a potential $-\lambda$. Neglecting the potentials, clearly $\psi_\lambda^1\left(\frac{\beta}{2}\right)$ and $\psi_\lambda^2\left(\frac{\beta}{2}\right)$ approach each other, and hence the denominator also approaches 1 in the same limit. Therefore, $g(\lambda)$ defines an everywhere-analytic function of λ which approaches the constant 1 at infinity, and now in all directions including the real axis, as it does so infinitesimally close to the real axis. By a theorem of complex analysis, a meromorphic function that approaches 1 in all directions at infinity must be equal to 1 everywhere

$$g(\lambda) = 1 \tag{3.75}$$

establishing Equation (3.71). Reorganizing the terms in Equation (3.71), formally we obtain

$$\frac{\det\left[-\frac{d^2}{d\tau^2} + W_1(\tau) - \lambda\right]}{\psi_\lambda^1\left(\frac{\beta}{2}\right)} = \frac{\det\left[-\frac{d^2}{d\tau^2} + W_2(\tau) - \lambda\right]}{\psi_\lambda^2\left(\frac{\beta}{2}\right)}, \tag{3.76}$$

where both sides are constants independent of the potentials W_i.

We now finally choose $\mathcal{N}$ by defining

$$\frac{\det\left[-\frac{d^2}{d\tau^2} + W(\tau)\right]}{\psi_0\left(\frac{\beta}{2}\right)} \equiv 2\pi\hbar\mathcal{N}^2 \tag{3.77}$$

and we will show that this choice is appropriate. Then

$$\mathcal{N}\det^{-\frac{1}{2}}\left[-\frac{d^2}{d\tau^2}+\omega^2\right]=\left(2\pi\hbar\psi_0^0\left(\tfrac{\beta}{2}\right)\right)^{-\frac{1}{2}}, \tag{3.78}$$

where $\psi_0^0(\tau)$ is the solution of Equation (3.69) for the free theory. It is easy to see that this solution is given by

$$\psi_0^0(\tau)=\frac{1}{\omega}\sinh\omega\left(\tau+\frac{\beta}{2}\right) \tag{3.79}$$

giving

$$\mathcal{N}\det^{\frac{-1}{2}}\left[-\frac{d^2}{d\tau^2}+\omega^2\right]=\left(2\pi\hbar\left(\frac{e^{\omega\beta}-e^{-\omega\beta}}{2\omega}\right)\right)^{-\frac{1}{2}}\approx\left(\frac{\omega}{\pi\hbar}\right)^{\frac{1}{2}}e^{-\omega\frac{\beta}{2}}. \tag{3.80}$$

We can compare this result with the direct calculation of the Euclidean persistence amplitude of the free harmonic oscillator. We find

$$\begin{aligned}\mathcal{N}\det^{-\frac{1}{2}}\left[-\frac{d^2}{d\tau^2}+\omega^2\right]&=\left\langle x=0\left|e^{-\frac{\beta}{\hbar}\left(-\frac{\hbar^2}{2}\frac{d^2}{dx^2}+\frac{1}{2}\omega^2x^2\right)}\right|x=0\right\rangle\\&=e^{-\frac{\beta E_0}{\hbar}}\langle x=0|\,E_0\rangle\langle E_0|\,x=0\rangle+\cdots,\end{aligned} \tag{3.81}$$

where $|E_0\rangle$ is the ground state. Clearly the normalized wave function is

$$\langle x|E_0\rangle=\left(\frac{\omega}{\pi\hbar}\right)^{\frac{1}{4}}e^{-\frac{\omega}{2\hbar}x^2} \tag{3.82}$$

while

$$E_0=\frac{1}{2}\hbar\omega \tag{3.83}$$

giving

$$\langle x=0|\,E_0\rangle=\left(\frac{\omega}{\pi\hbar}\right)^{\frac{1}{4}}. \tag{3.84}$$

Hence Equation (3.81) yields

$$\mathcal{N}\det^{-\frac{1}{2}}\left[-\frac{d^2}{d\tau^2}+\omega^2\right]=\left(\frac{\omega}{\pi\hbar}\right)^{\frac{1}{2}}e^{-\omega\frac{\beta}{2}} \tag{3.85}$$

in agreement with Equation (3.80), and confirming the definition of the normalization $\mathcal{N}$ chosen in Equation (3.77).

3.5.2 Evaluation of K

Finally we must evaluate the factor K. K is given by the ratio

$$\frac{1}{K^2}=\frac{\det'\left[-\frac{d^2}{d\tau^2}+V''(\bar{z}(\tau-\tau_1)\right]}{\det\left[-\frac{d^2}{d\tau^2}+\omega^2\right]} \tag{3.86}$$

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from Equations (3.64) and (3.66) for $n=0$. Thus

$$\frac{1}{K^2} = \left(\frac{\psi_0\left(\frac{\beta}{2}\right)/\lambda_0}{\psi_0^0\left(\frac{\beta}{2}\right)} \right), \tag{3.87}$$

where λ_0 is the smallest eigenvalue in the presence of an instanton. To calculate $\psi_0\left(\frac{\beta}{2}\right)$ and λ_0 approximately we describe again the procedure given in Coleman [31]. First we need to solve

$$\left(-\partial_\tau^2 + V''(\bar{z}(\tau))\right)\psi_0(\tau) = 0 \tag{3.88}$$

with the boundary conditions $\psi_0(-\beta/2) = 0$ and $\partial_\tau\psi_0(-\beta/2) = 1$. We already know one solution of Equation (3.88), albeit one that does not satisfy the boundary conditions: the zero mode of the operator in Equation (3.30) due to time translation invariance, we will call it here $x_1(\tau)$:

$$x_1(\tau) = \frac{1}{\sqrt{S_0}}\frac{d\bar{z}}{d\tau}. \tag{3.89}$$

$x_1(\tau) \to Ae^{-\omega|\tau|}$ as $\tau \to \pm\infty$. A is determined by the equation of motion, Equation (3.30), which integrated once corresponds to

$$\dot{\bar{z}}(\tau) = \sqrt{2V(\bar{z}(\tau))}. \tag{3.90}$$

Once we have A we can compute $\psi(\frac{\beta}{2})$ and λ_0.

We know that there must exist a second independent solution of the differential Equation (3.88), $y_1(\tau)$ which we normalize so that the Wronskian

$$x_1\frac{dy_1}{d\tau} - y_1\frac{dx_1}{d\tau} = 2A^2. \tag{3.91}$$

We remind the reader that the Wronskian between two linearly independent solutions of a linear second-order differential equation is non-zero, and with no first derivative term, as in Equation (3.88), is a constant. Then as $\tau \to \pm\infty$ we have

$$\dot{y}_1(\tau) \pm \omega y_1(\tau) = 2A\omega e^{\omega|\tau|} \tag{3.92}$$

using the known behaviour of $x_1(\tau)$. The general solution of Equation (3.92) is any particular solution plus an arbitrary factor times the homogeneous solution

$$y_1(\tau) = \pm Ae^{\omega|\tau|} + Be^{\mp\omega|\tau|}, \tag{3.93}$$

where B is an arbitrary constant. Evidently the homogenous solution is a negligible perturbation on the particular solution, and $y_1(\tau) \to \pm Ae^{\omega|\tau|}$ as $\tau \to \pm\infty$. Then we construct $\psi_0(\tau)$ as

$$\psi_0(\tau) = \frac{1}{2\omega A}\left(e^{\omega\beta/2}x_1(\tau) + e^{-\omega\beta/2}y_1(\tau)\right), \tag{3.94}$$

verifying

$$\psi_0(-\beta/2) = \frac{1}{2\omega A}\left(e^{\omega\beta/2}x_1(-\beta/2) + e^{-\omega\beta/2}y_1(-\beta/2)\right)$$
$$\approx \frac{1}{2\omega A}\left(e^{\omega\beta/2}Ae^{-\omega\beta/2} + e^{-\omega\beta/2}(-A)e^{\omega\beta/2}\right) = 0 \qquad (3.95)$$

while

$$\left.\frac{d\psi_0(-\beta/2)}{d\tau}\right|_{\frac{-\beta}{2}} \approx \frac{1}{2\omega A}\left(e^{\omega\beta/2}\left.\frac{d}{d\tau}Ae^{\omega\tau}\right|_{\frac{-\beta}{2}} + e^{-\omega\beta/2}\left.\frac{d}{d\tau}(-A)e^{-\omega\tau}\right|_{\frac{-\beta}{2}}\right) = 1. \qquad (3.96)$$

Then it is also easy to see

$$\psi_0(\beta/2) = \frac{1}{\omega}, \qquad (3.97)$$

which we will need later.

We also need to calculate the smallest eigenvalue λ_0 of Equation (3.69). To do this we convert the differential equation to an integral equation using the corresponding Green function. The Green function satisfying the appropriate boundary conditions is constructed from $x_1(\tau)$ and $y_1(\tau)$ using standard techniques and is given by

$$G(\tau,\tau') = \begin{cases} \frac{1}{2A^2}(-y_1(\tau')x_1(\tau) + x_1(\tau')y_1(\tau)) & \tau > \tau' \\ 0 & \tau < \tau' \end{cases}. \qquad (3.98)$$

Then the differential equation is converted to an integral equation

$$\psi_\lambda(\tau) = \psi_0(\tau) + \frac{\lambda}{2A^2}\int_{\frac{-\beta}{2}}^{\tau} d\tau'(x_1(\tau')y_1(\tau) - y_1(\tau')x_1(\tau))\psi_\lambda(\tau')$$
$$\approx \psi_0(\tau) + \frac{\lambda}{2A^2}\int_{\frac{-\beta}{2}}^{\tau} d\tau'(x_1(\tau')y_1(\tau) - y_1(\tau')x_1(\tau))\psi_0(\tau'). \qquad (3.99)$$

This wave function vanishes for the lowest eigenvalue λ_0 (and actually for all eigenvalues λ_n) at $\tau = \beta/2$ by Equation (3.70), thus

$$\psi_0(\beta/2) + \frac{\lambda}{2A^2}\int_{\frac{-\beta}{2}}^{\frac{\beta}{2}} d\tau'(x_1(\tau')y_1(\beta/2) - y_1(\tau')x_1(\beta/2))\psi_0(\tau')$$
$$\approx \frac{1}{\omega} - \frac{\lambda}{2A^2}\int_{\frac{-\beta}{2}}^{\frac{\beta}{2}} d\tau'(x_1(\tau')y_1(\beta/2) - y_1(\tau')x_1(\beta/2))$$
$$\frac{1}{2\omega A}\left(e^{\omega\beta/2}x_1(\tau') + e^{-\omega\beta/2}y_1(\tau')\right)$$
$$\approx \frac{1}{\omega} - \frac{\lambda}{2A^2}\int_{\frac{-\beta}{2}}^{\frac{\beta}{2}} d\tau'(x_1(\tau')e^{\omega\beta/2} - y_1(\tau')e^{-\omega\beta/2})$$
$$\frac{1}{2\omega}\left(e^{\omega\beta/2}x_1(\tau') + e^{-\omega\beta/2}y_1(\tau')\right)$$

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$$\approx \frac{1}{\omega} - \frac{\lambda}{2A^2\omega}\int_{\frac{-\beta}{2}}^{\frac{\beta}{2}} d\tau'(x_1^2(\tau')e^{\omega\beta} - y_1^2(\tau')e^{-\omega\beta})$$
$$\approx \frac{1}{\omega} - \frac{\lambda}{4A^2\omega}\int_{\frac{-\beta}{2}}^{\frac{\beta}{2}} d\tau' x_1^2(\tau')e^{\omega\beta} = \frac{1}{\omega} - \frac{\lambda}{4A^2\omega}e^{\omega\beta} = 0. \tag{3.100}$$

In the penultimate equation, we can drop the second term because it behaves at most as $\sim\beta$, since $y_1(\tau)\sim e^{\beta/2}$ at the boundaries of the integration domain at $\pm\beta/2$, while the first term behaves as $\sim e^{\beta}$ since $\int x_1^2(\tau)d\tau$ is normalized to 1. This gives quite simply

$$\lambda_0 \approx 4A^2 e^{-\omega\beta}. \tag{3.101}$$

Then finally we get

$$K = \left(\frac{\psi_0^0\left(\beta/2\right)}{\psi_0\left(\beta/2\right)/\lambda_0}\right)^{\frac{1}{2}} = \frac{e^{\omega\beta}/2\omega}{(1/\omega 4A^2 e^{-\omega\beta})} = 2A^2. \tag{3.102}$$

Thus we have found that the matrix element

$$\langle a|e^{-\beta\hat{h}(\hat{X},\hat{P})/\hbar}|-a\rangle = \sinh\left(\left(\frac{S_0}{2\pi\hbar}\right)^{\frac{1}{2}} e^{-S_0/\hbar}2A^2\beta\right)\left(\frac{\omega}{\pi\hbar}\right)^{\frac{1}{2}} e^{-\omega\frac{\beta}{2}}. \tag{3.103}$$

To see explicitly see how to compute A, we can consider a convenient, completely integrable example, $V(x) = (\gamma^2/2)(x^2-a^2)^2$, which has $\omega^2 = V''(\pm a) = (2\gamma a)^2$. Then Equation (3.30) yields

$$\int_0^{\bar{z}(\tau-\tau_1)} \frac{dz}{\gamma(z^2-a^2)} = \tau - \tau_1 \tag{3.104}$$

with exact solution

$$\bar{z}(\tau) = a\tanh(a\gamma(\tau-\tau_1)). \tag{3.105}$$

Thus A is determined by

$$x_1(\tau) = \frac{\dot{\bar{z}}(\tau)}{\sqrt{S_0}} = \frac{a^2\gamma}{\sqrt{S_0}\cosh^2(a\gamma(\tau-\tau_1))}, \tag{3.106}$$

which behaves as

$$\lim_{\tau\to\pm\infty} x_1(\tau) = \frac{4a^2\gamma}{\sqrt{S_0}}e^{-2a\gamma|\tau|} = \frac{2a\omega}{\sqrt{S_0}}e^{-\omega|\tau|} = Ae^{-\omega|\tau|}. \tag{3.107}$$

$\sqrt{S_0}$ is calculated from Equation (3.27), giving

$$S_0 = \int_{-a}^{a} dz\gamma(z^2-a^2) = \frac{4}{3}\gamma a^3 = \frac{2}{3}\omega a^2. \tag{3.108}$$

Hence $A = \frac{2a\omega}{\sqrt{(2/3)\omega a^2}} = \sqrt{\frac{6}{\omega}}$, for this example.

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3.6 Extracting the Lowest Energy Levels

On the other hand, the matrix element of Equation (3.103) can be evaluated by inserting a complete set of energy eigenstates between the operator and the position eigenstates on the left-hand side, yielding

$$\langle a|e^{-\beta\hat{h}(\hat{X},\hat{P})/\hbar}|-a\rangle = e^{-\beta E_0/\hbar}\langle a|E_0\rangle\langle E_0|-a\rangle + e^{-\beta E_1/\hbar}\langle a|E_1\rangle\langle E_1|-a\rangle + \cdots, \tag{3.109}$$

where we have explicitly written only the first two terms as we expect that the two classical states, $|\pm a\rangle$, are reorganized due to tunnelling into the two lowest-lying states, $|E_0\rangle$ and $|E_1\rangle$. Indeed, comparing Equation (3.103) and Equation (3.109) we find

$$E_0 = \frac{\hbar}{2}\omega - \hbar\left(\frac{S_0}{2\pi\hbar}\right)^{\frac{1}{2}} e^{-S_0/\hbar}2A^2 \tag{3.110}$$

while

$$E_1 = \frac{\hbar}{2}\omega + \hbar\left(\frac{S_0}{2\pi\hbar}\right)^{\frac{1}{2}} e^{-S_0/\hbar}2A^2. \tag{3.111}$$

It should be stressed that our calculation is only valid for the energy difference, not for the corrections to the energies directly. Indeed, there are ordinary perturbative corrections to the energy levels which are normally far greater than the non-perturbative, exponentially suppressed correction that we have calculated. However, none of these perturbative corrections can see any tunnelling phenomena. Thus our calculation gives the leading term in the correction due to tunnelling. Thus, the energy splitting which relies on tunnelling is found only through our calculation, and not through perturbative calculations.

We also find the relations

$$\langle a|E_0\rangle\langle E_0|-a\rangle = \left(\frac{\omega}{\pi\hbar}\right)^{\frac{1}{2}} \tag{3.112}$$

in addition to

$$\langle a|E_1\rangle\langle E_1|-a\rangle = -\left(\frac{\omega}{\pi\hbar}\right)^{\frac{1}{2}} \tag{3.113}$$

while a simple adaptation of our analysis yields

$$\langle a|E_0\rangle\langle E_0|a\rangle = \left(\frac{\omega}{\pi\hbar}\right)^{\frac{1}{2}} \tag{3.114}$$

in addition to

$$\langle a|E_1\rangle\langle E_1|a\rangle = \left(\frac{\omega}{\pi\hbar}\right)^{\frac{1}{2}}. \tag{3.115}$$

These yield $\langle E_0|-a\rangle = \langle E_0|a\rangle$ while $\langle E_1|-a\rangle = -\langle E_1|a\rangle$ which are consistent with $|E_0\rangle$ being an even function, *i.e.* $|E_0\rangle$ being an even superposition of the position eigenstates $|a\rangle$ and $|-a\rangle$ while $|E_1\rangle$ being an odd function and hence an odd superposition of these two position eigenstates.

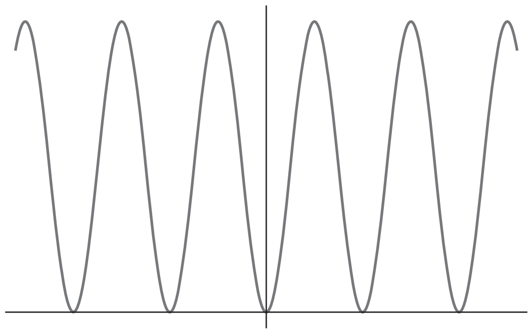

Figure 3.7. A generic periodic potential with minima occurring at na with $n \in \mathbb{Z}$, where a is the distance between neighbouring minima

3.7 Tunnelling in Periodic Potentials

We will end this chapter with an application of the method to periodic potentials. Periodic potentials are very important in condensed matter physics, as crystal lattices are well-approximated by the theory of electrons in a periodic potential furnished by the atomic nuclei. The idea is easiest to enunciate in a one-dimensional example. Consider a potential of the form given in Figure 3.7. A particle in the presence of such a potential with minimal energy will classically, certainly, be localized in the bottom of the wells of the potential. If there is no tunnelling, there would be an infinite number of degenerate states corresponding to the state where the particle is localized in state labelled by integer $n \in \mathbb{Z}$. This could also be a very large, finite number of minima. However, quantum tunnelling will completely change the spectrum. Just as in the case of the double well potential, the states will reorganize so that the most symmetric superposition will correspond to the true ground state, and various other superpositions will give rise to excited states, albeit with excitation energies proportional to the tunnelling amplitude. The tunnelling amplitude is expected to be exponentially small and non-perturbative in the coupling constant.

As in the case of the double well potential, the instanton trajectories will correspond to solutions of the analogous dynamical problem in the inverted potential in Euclidean time (as depicted in Figure 3.8), where the trajectories commence at the top of a potential hill, stay there for a long time, then quickly fall through the minimum of the inverted potential, and then arrive at the top of the adjacent potential hill, and stay there for the remaining positive Euclidean time.

For the simple, real-time Lagrangian

$$L = \frac{1}{2}\dot{x}^2 - V(x), \tag{3.116}$$

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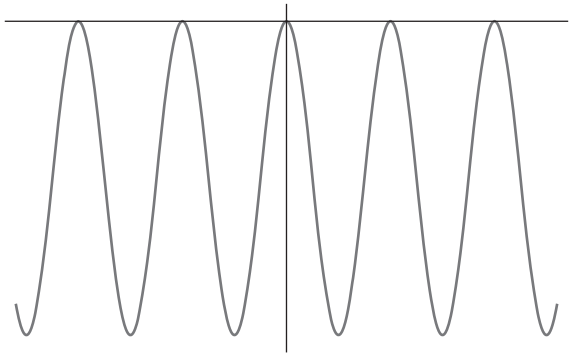

Figure 3.8. The inverted generic periodic potential with maxima occurring at na with $n \in \mathbb{Z}$

where $\dot{x} = \frac{dx(t)}{dt}$, while the Euclidean Lagrangian is simply

$$L = \frac{1}{2}\dot{x}^2 + V(x), \tag{3.117}$$

where $\dot{x} = \frac{dx(\tau)}{d\tau}$. As $V(na) = 0$ for $n \in \mathbb{Z}$, we impose the boundary conditions $x(\tau = -\infty) = na$ but $x(\tau = \infty) = (n+1)a$ for an instanton and $x(\tau = \infty) = (n-1)a$ for an anti-instanton and look for solutions of the Euclidean equations of motion

$$\frac{d^2x(\tau)}{d\tau^2} - V'(x(\tau)) = 0. \tag{3.118}$$

This immediately affords a first integral; multiplying by $\dot{x}(\tau)$ and integrating gives

$$\frac{1}{2}\dot{x}^2(\tau) - V(x(\tau)) = 0, \tag{3.119}$$

where we have fixed the constant with the boundary conditions. This equation admits a solution in general, the instanton, but it does depend on the explicit details of the potential. However, we can find the action of the corresponding instanton, which only depends on an integral of the potential, by first isolating

$$\dot{x} = \sqrt{2V(x)}, \tag{3.120}$$

and then

$$\begin{aligned} S_0 &= \int_{-\infty}^{\infty} d\tau \frac{1}{2}\dot{x}^2 + V(x) = \int_{-\infty}^{\infty} d\tau \left(\frac{1}{2}\dot{x}\sqrt{2V(x)} + \frac{1}{2}\dot{x}\sqrt{2V(x)} \right) \\ &= \int_{na}^{(n+1a} dx \sqrt{2V(x)}. \end{aligned} \tag{3.121}$$

Although we may naively want to compute the amplitude for tunnelling between neighbouring vacua, it is actually more informative to compute the amplitude for a transition from vacuum n to vacuum $n+m$. Naively we would

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approximate this amplitude by summing over any number of pairs of widely separated instanton anti-instanton configurations appended by a string of m instantons. However, this logic would be faulty. There is no reason to restrict the order of the instantons and anti-instantons except that they should tunnel from the immediately preceding vacuum to an adjacent vacuum, and finally we should arrive at the minimum indexed by $n+m$. Thus, one can choose the instantons or anti-instantons in any order, as long as they start at n and end at $n+m$. This means that if there are N instantons, which must be greater than m, then there must be $N-m$ anti-instantons. Thus there are as many distinct paths of instantons as there are ways to order N plus signs and $N-m$ minus signs. This gives a degeneracy factor of

$$\frac{(2N-m)!}{N!(N-m)!}. \tag{3.122}$$

Furthermore, when we integrate over the Gaussian fluctuations for each instanton or anti-instanton, we get the usual determinantal factor K for each instanton or anti-instanton, but we do encounter one zero mode corresponding to each one's position, which we omit in the determinant. Then we integrate over the positions of the instantons and anti-instantons, except that the position of each instanton or anti-instanton must occur at the position after the preceding one, as the instantons and anti-instantons correspond to specific tunnelling between specific vacua. This gives the integral

$$\int_{-\beta/2}^{\beta/2} d\tau_1 \int_{\tau_1}^{\beta/2} d\tau_2 \cdots \int_{\tau_{2N-1}}^{\beta/2} d\tau_{2N-m} = \frac{\beta^{2N-m}}{(2N-m)!}. \tag{3.123}$$

As usual, the action for any instanton or anti-instanton is the same and equal to S_0. Thus, for N instantons and $N-m$ anti-instantons we get

$$\langle n+m|e^{-\beta\hat{h}(\hat{X},\hat{P})/\hbar}|n\rangle = \sum_{N=m}^{\infty} e^{-(2N-m)S_0/\hbar} K^{2N-m} \frac{(2N-m)!}{N!(N-m)!} \frac{\beta^{2N-m}}{(2N-m)!}. \tag{3.124}$$

This sum is unclear for identifying the underlying spectrum and the contribution of each energy eigenstate; however, if we re-write the sum as a double sum over N instantons and M anti-instantons with a constraint $M = N-m$ we have

$$\langle n+m|e^{-\beta\hat{h}(\hat{X},\hat{P})/\hbar}|n\rangle = \left(\frac{\omega}{\pi\hbar}\right)^{1/2} e^{-\beta\omega/2} \times \sum_{N,M=0}^{\infty} e^{-(N+M)S_0/\hbar} K^{N+M} \frac{\beta^{N+M}}{N!M!} \delta_{N-m,M}, \tag{3.125}$$

where $\omega^2 = V''(na)$. Now the Kronecker delta can be expressed via its Fourier series as

$$\delta_{N-m,M} = \int_0^{2\pi} \frac{d\theta}{2\pi} e^{i\theta(N-m-M)} \tag{3.126}$$

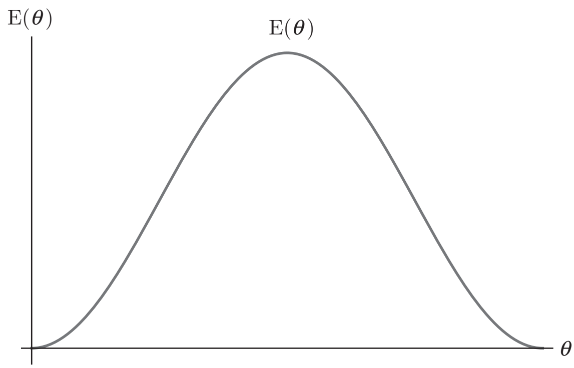

Figure 3.9. The energy band as a function of θ

and so we easily find

$$
\begin{aligned}
&\langle n+m|e^{-\beta\hat{h}(\hat{X},\hat{P})/\hbar}|n\rangle = \\
&= \left(\frac{\omega}{\pi\hbar}\right)^{1/2} e^{-\beta\omega/2}\int_0^{2\pi}\frac{d\theta}{2\pi}\sum_{N,M=1}^{\infty}\frac{(K\beta e^{-S_0/\hbar})^{N+M}}{N!M!}e^{i\theta(N-m-M)} \\
&= \left(\frac{\omega}{\pi\hbar}\right)^{1/2} e^{-\beta\omega/2}\int_0^{2\pi}\frac{d\theta}{2\pi}e^{-im\theta}\sum_{N,M=1}^{\infty}\frac{(K\beta e^{-S_0/\hbar})^{N+M}}{N!M!}e^{i\theta(N-M)} \\
&= \left(\frac{\omega}{\pi\hbar}\right)^{1/2} e^{-\beta\omega/2}\int_0^{2\pi}\frac{d\theta}{2\pi}e^{-im\theta}e^{\left(K\beta e^{-S_0/\hbar}e^{i\theta}\right)}e^{\left(K\beta e^{-S_0/\hbar}e^{-i\theta}\right)} \\
&= \left(\frac{\omega}{\pi\hbar}\right)^{1/2} e^{-\beta\omega/2}\int_0^{2\pi}\frac{d\theta}{2\pi}e^{-im\theta}e^{\left(K\beta e^{-S_0/\hbar}\left(e^{i\theta}+e^{-i\theta}\right)\right)} \\
&= \left(\frac{\omega}{\pi\hbar}\right)^{1/2} e^{-\beta\omega/2}\int_0^{2\pi}\frac{d\theta}{2\pi}e^{-im\theta}e^{\left(2K\beta e^{-S_0/\hbar}\cos\theta\right)}.
\end{aligned}
\tag{3.127}
$$

But this expression for the matrix element has a clear interpretation in terms of the spectrum. We see that the spectrum has become a continuum, parametrized by θ. If we write

$$\langle n+m|e^{-\beta\hat{h}(\hat{X},\hat{P})/\hbar}|n\rangle = \int_0^{2\pi}\frac{d\theta}{2\pi}e^{-\beta E(\theta)/\hbar}\langle n+m|E(\theta)\rangle\langle E(\theta)|n\rangle \tag{3.128}$$

we identify

$$E(\theta) = \hbar\omega/2 - 2\hbar K e^{-S_0/\hbar}\cos\theta \tag{3.129}$$

and

$$\langle n+m|E(\theta)\rangle\langle E(\theta)|n\rangle = \left(\frac{\omega}{\pi\hbar}\right)^{1/2}\frac{e^{-im\theta}}{2\pi}, \tag{3.130}$$

which affords the identification

$$\langle n|E(\theta)\rangle = \left(\frac{\omega}{\pi\hbar}\right)^{1/4}\frac{e^{-in\theta}}{\sqrt{2\pi}}. \tag{3.131}$$

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Thus our infinitely degenerate spectrum of discrete classical vacua has turned into a continuum of states, what is called a band in condensed matter physics, with an energy that varies as $\cos\theta$, as depicted in Figure 3.9. The states are now in a continuum, and hence must be normalized in the sense of a Dirac delta function rather than a Kronecker delta. The amplitude of the band $2\hbar K e^{-S_0/\hbar}$ contains the tell-tale factor of the exponential of minus the Euclidean action, the hallmark of a tunnelling amplitude.

We will see in future chapters that periodic potentials appear commonly and play an important role in various instanton calculations.