Aevo rarissima nostro, simplicitas
Simplicity, a very rare thing in our age
OVID (43 BC–17), Ars Amatoria, Book 1, 241

6

Path Integrals with Topological Constraints

The path integral representations of the time evolution amplitudes considered so far were derived for orbits $x(t)$ fluctuating in Euclidean space with Cartesian coordinates. Each coordinate runs from minus infinity to plus infinity. In many physical systems, however, orbits are confined to a topologically restricted part of a Cartesian coordinate system. This changes the quantum-mechanical completeness relation and with it the derivation of the path integral from the time-sliced time evolution operator in Section 2.1. We shall consider here only a point particle moving on a circle, in a half-space, or in a box. The path integral treatment of these systems is the prototype for any extension to more general topologies.

6.1 Point Particle on Circle

For a point particle on a circle, the orbits are specified in terms of an angular variable $\varphi(t) \in [0, 2\pi]$ subject to the topological constraint that $\varphi = 0$ and $\varphi = 2\pi$ be identical points.

The initial step in the derivation of the path integral for such a system is the same as before: The time evolution operator is decomposed into a product

$$\langle \varphi_b t_b | \varphi_a t_a \rangle = \langle \varphi_b | \exp\left[-\frac{i}{\hbar}(t_b - t_a)\hat{H}\right] |\varphi_a\rangle \equiv \langle \varphi_b | \prod_{n=1}^{N+1} \exp\left(-\frac{i}{\hbar}\epsilon\hat{H}\right) |\varphi_a\rangle. \tag{6.1}$$

The restricted geometry shows up in the completeness relations to be inserted between the factors on the right-hand side for $n = 1, \ldots, N$:

$$\int_0^{2\pi} d\varphi_n |\varphi_n\rangle\langle\varphi_n| = 1. \tag{6.2}$$

If the integrand is singular at $\varphi = 0$, the integrations must end at an infinitesimal piece below 2π. Otherwise there is the danger of double-counting the contributions from the identical points $\varphi = 0$ and $\varphi = 2\pi$. The orthogonality relations on these intervals are

$$\langle \varphi_n | \varphi_{n-1} \rangle = \delta(\varphi_n - \varphi_{n-1}), \quad \varphi_n \in [0, 2\pi). \tag{6.3}$$

The δ-function can be expanded into a complete set of periodic functions on the circle:

$$\delta\left(\varphi_n-\varphi_{n-1}\right)=\sum_{m_n=-\infty}^{\infty}\frac{1}{2\pi}\exp[im_n(\varphi_n-\varphi_{n-1})]. \tag{6.4}$$

For a trivial system with no Hamiltonian, the scalar products (6.4) lead to the following representation of the transition amplitude:

$$(\varphi_b t_b|\varphi_a t_a)_0=\prod_{n=1}^{N}\left[\int_0^{2\pi}d\varphi_n\right]\prod_{n=1}^{N+1}\left[\sum_{m_n}\frac{1}{2\pi}\right]\exp\left[i\sum_{n=1}^{N+1}m_n(\varphi_n-\varphi_{n-1})\right]. \tag{6.5}$$

We now introduce a Hamiltonian $H(p,\varphi)$. At each small time step, we calculate

$$\begin{aligned}(\varphi_n t_n|\varphi_{n-1}t_{n-1}) &= \langle\varphi_n|\exp\left[-\frac{i}{\hbar}\epsilon\hat{H}(p,\varphi)\right]|\varphi_{n-1}\rangle\\ &= \exp\left[-\frac{i}{\hbar}\epsilon\hat{H}(-i\hbar\partial_{\varphi_n},\varphi_n)\right]\langle\varphi_n|\varphi_{n-1}\rangle.\end{aligned}$$

Replacing the scalar products by their spectral representation (6.4), this becomes

$$\begin{aligned}(\varphi_n t_n|\varphi_{n-1}t_{n-1}) &= \langle\varphi_n|\exp\left[-\frac{i}{\hbar}\epsilon\hat{H}(p,\varphi)\right]|\varphi_{n-1}\rangle\\ &= \exp\left[-\frac{i}{\hbar}\epsilon\hat{H}(-i\hbar\partial_{\varphi_n},\varphi_n)\right]\sum_{m_n=-\infty}^{\infty}\frac{1}{2\pi}\exp[im_n(\varphi_n-\varphi_{n-1})].\end{aligned} \tag{6.6}$$

By applying the operator in front of the sum to each term, we obtain

$$(\varphi_n\, t_n|\varphi_{n-1}\, t_{n-1})=\sum_{m_n=-\infty}^{\infty}\frac{1}{2\pi}\exp\left[im_n(\varphi_n-\varphi_{n-1})-\frac{i\epsilon}{\hbar}H(\hbar m_n,\varphi_n)\right]. \tag{6.7}$$

The total amplitude can therefore be written as

$$\begin{aligned}(\varphi_b t_b|\varphi_a t_a) \;\approx\; &\prod_{n=1}^{N}\left[\int_0^{2\pi}d\varphi_n\right]\prod_{n=1}^{N+1}\left[\sum_{m_n=-\infty}^{\infty}\frac{1}{2\pi}\right]\\ &\times\exp\left\{i\sum_{n=1}^{N+1}\left[m_n(\varphi_n-\varphi_{n-1})-\frac{1}{\hbar}\epsilon H(\hbar m_n,\varphi_n)\right]\right\}.\end{aligned} \tag{6.8}$$

This is the desired generalization of the original path integral from Cartesian to cyclic coordinates. As a consequence of the indistinguishability of $\varphi(t)$ and $\varphi(t)+2\pi n$, the momentum integrations have turned into sums over integer numbers. The sums reflect the fact that the quantum-mechanical wave functions $(1/\sqrt{2\pi})\exp(ip_\varphi\varphi/\hbar)$ are single-valued.

The discrete momenta enter into (6.8) via a "momentum step sum" rather than a proper path integral. At first sight, such an expression looks somewhat hard to deal with in practical calculations. Fortunately, it can be turned into a more comfortable equivalent form, involving a proper continuous path integral. This is possible at the expense of a single additional infinite sum which guarantees the cyclic invariance in the variable φ. To find the equivalent form, we recall Poisson's formula (1.197),

$$\sum_{l=-\infty}^{\infty} e^{2\pi ikl} = \sum_{m=-\infty}^{\infty} \delta(k-m), \tag{6.9}$$

to make the right-hand side of (6.4) a periodic sum of δ-functions, so that (6.3) becomes

$$\langle\varphi_n|\varphi_{n-1}\rangle = \sum_{l=-\infty}^{\infty} \delta(\varphi_n - \varphi_{n-1} + 2\pi l). \tag{6.10}$$

A Fourier decomposition of the δ-functions yields

$$\langle\varphi_n|\varphi_{n-1}\rangle = \sum_{l=-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{dk_n}{2\pi} \exp[ik_n(\varphi_n - \varphi_{n-1}) + 2\pi ik_n l]. \tag{6.11}$$

Note that the right-hand side reduces to (6.4) when applying Poisson's summation formula (6.9) to the l-sum, which produces a sum of δ-functions for the integer values of $k_n = m_n = 0, \pm 1, \pm 2, \dots$. Using this expansion rather than (6.4), the amplitude (6.5) with no Hamiltonian takes the form

$$(\varphi_b t_b|\varphi_a t_a)_0 = \prod_{n=1}^{N}\left[\int_0^{2\pi} d\varphi_n\right] \prod_{n=1}^{N+1}\left[\int_{-\infty}^{\infty} \frac{dk_n}{2\pi} \sum_{l_n=-\infty}^{\infty}\right] e^{i\sum_{n=1}^{N+1}[k_n(\varphi_n-\varphi_{n-1})+2\pi k_n l_n]}. \tag{6.12}$$

In this expression, we observe that the sums over l_n can be absorbed into the variables φ_n by extending their range of integration from $[0, 2\pi)$ to $(-\infty, \infty)$. Only in the last sum $\sum_{l_{N+1}}$, this is impossible, and we arrive at

$$(\varphi_b t_b|\varphi_a t_a)_0 = \sum_{l=-\infty}^{\infty} \prod_{n=1}^{N}\left[\int_{-\infty}^{\infty} d\varphi_n\right] \prod_{n=1}^{N+1}\left[\int_{-\infty}^{\infty} \frac{dk_n}{2\pi}\right] e^{i\sum_{n=1}^{N+1} k_n(\varphi_n-\varphi_{n-1}+2\pi l\delta_{n,N+1})}. \tag{6.13}$$

The right-hand side looks just like an $\hat{H} \equiv 0$ -amplitude of an ordinary particle which would read

$$(\varphi_b t_b|\varphi_a t_a)_{0,\text{noncyclic}} = \prod_{n=1}^{N}\left[\int_{-\infty}^{\infty} d\varphi_n\right] \prod_{n=1}^{N+1}\left[\int_{-\infty}^{\infty} \frac{dk_n}{2\pi}\right] e^{i\sum_{n=1}^{N+1} k_n(\varphi_n-\varphi_{n-1})}. \tag{6.14}$$

The amplitude (6.13) differs from this by the sum over paths running over all periodic repetitions of the final point $\varphi_b + 2\pi n, t_b$. The amplitude (6.13) may therefore be written as a sum over all periodically repeated final points of the amplitude (6.14):

$$(\varphi_b t_b|\varphi_a t_a)_0 = \sum_{l=-\infty}^{\infty} (\varphi_b + 2\pi l, t_b|\varphi_a t_a)_{0,\text{noncyclic}}\,. \tag{6.15}$$

In each term on the right-hand side, the Hamiltonian can be inserted as usual, and we arrive at the time-sliced formula

$$(\varphi_b t_b|\varphi_a t_a) \approx \sum_{l=-\infty}^{\infty} \prod_{n=1}^{N} \left[\int_{-\infty}^{\infty} d\varphi_n\right] \prod_{n=1}^{N+1} \left[\int_{-\infty}^{\infty} \frac{dp_n}{2\pi\hbar}\right]$$
$$\times \exp\left\{\frac{i}{\hbar}\sum_{n=1}^{N+1}\left[p_n(\varphi_n-\varphi_{n-1}+2\pi l\delta_{n,N+1})-\epsilon H(p_n,\varphi_n)\right]\right\}. \tag{6.16}$$

In the continuum limit, this tends to the path integral

$$(\varphi_b t_b|\varphi_a t_a) \xrightarrow{\epsilon\to 0} \sum_{l=-\infty}^{\infty} \int_{\varphi_a\rightsquigarrow\varphi_b+2\pi l} \mathcal{D}\varphi(t) \int \frac{\mathcal{D}p(t)}{2\pi\hbar} \exp\left\{\frac{i}{\hbar}\int_{t_a}^{t_b} dt[p\dot\varphi - H(p,\varphi)]\right\}. \tag{6.17}$$

The way in which this path integral has replaced the sum over all paths on the circle $\varphi \in [0, 2\pi)$ by the sum over all paths with the same action on the entire φ-axis is illustrated in Fig. 6.1.

As an example, consider a free particle moving on a circle with a Hamiltonian

$$H(p,\varphi) = \frac{p^2}{2M}. \tag{6.18}$$

The ordinary noncyclic path integral is

$$(\varphi_b t_b|\varphi_a t_a)_{\rm noncyclic} = \frac{1}{\sqrt{2\pi\hbar i(t_b-t_a)/M}} \exp\left[\frac{i}{\hbar}\frac{M}{2}\frac{(\varphi_b-\varphi_a)^2}{t_b-t_a}\right]. \tag{6.19}$$

Using Eq. (6.15), the cyclic amplitude is given by the periodic Gaussian

$$(\varphi_b t_b|\varphi_a t_a) = \frac{1}{\sqrt{2\pi\hbar i(t_b-t_a)/M}} \sum_{l=-\infty}^{\infty} \exp\left[\frac{i}{\hbar}\frac{M}{2}\frac{(\varphi_b-\varphi_a+2\pi l)^2}{t_b-t_a}\right]. \tag{6.20}$$

The same amplitude could, of course, have been obtained by a direct quantum-mechanical calculation based on the wave functions

$$\psi_m(\varphi) = \frac{1}{\sqrt{2\pi}} e^{im\varphi} \tag{6.21}$$

and the energy eigenvalues

$$H = \frac{\hbar^2}{2M} m^2. \tag{6.22}$$

Within operator quantum mechanics, we find

$$\begin{aligned}
(\varphi_b t_b|\varphi_a t_a) &= \langle\varphi_b|\exp\left[-\frac{i}{\hbar}(t_b-t_a)\hat H\right]|\varphi_a\rangle \\
&= \sum_{m=-\infty}^{\infty} \psi_m(\varphi_b)\psi_m^*(\varphi_a)\exp\left[-\frac{i}{\hbar}\frac{\hbar^2 m^2}{2M}(t_b-t_a)\right] \\
&= \sum_{m=-\infty}^{\infty} \frac{1}{2\pi}\exp\left[im(\varphi_b-\varphi_a) - i\frac{\hbar m^2}{2M}(t_b-t_a)\right].
\end{aligned} \tag{6.23}$$

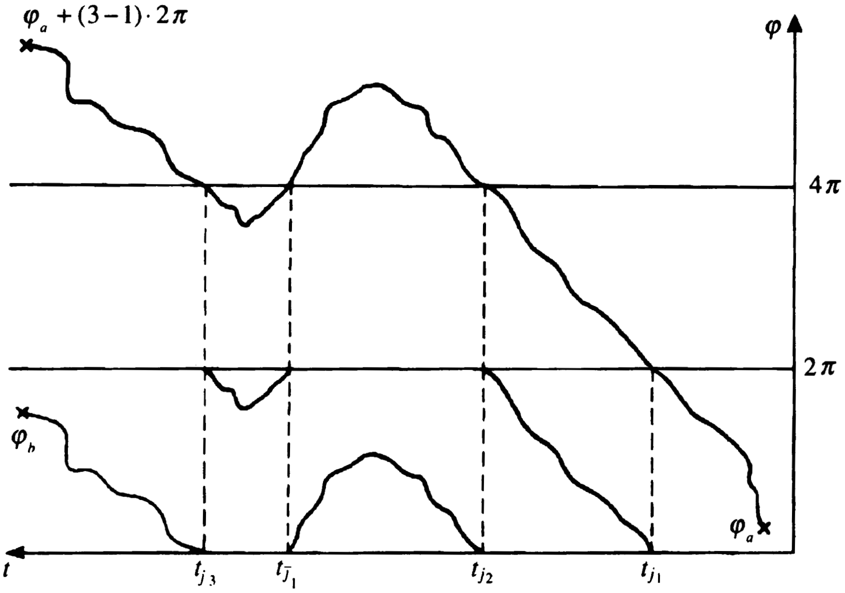


Figure 6.1 Path with 3 jumps from 2π to 0 at t_{j1}, t_{j2}, t_{j3}, and with one jump from 0 to 2π at $t_{\bar{j}1}$. It can be drawn as a smooth path in the *extended zone scheme*, arriving at $\varphi^{(n,\bar{n})} = \varphi_b + (n - \bar{n})2\pi$, where n and $\bar{n}$ count the number of jumps of the first and the second type, respectively.

If the sum over m is converted into an integral over p and a dual l-sum via Poisson's formula (6.9), this coincides with the previous result:

$$\begin{aligned}(\varphi_b t_b|\varphi_a t_a) &= \sum_{l=-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar} \exp\left\{\frac{i}{\hbar}\left[p(\varphi_b - \varphi_a + 2\pi l) - \frac{p^2}{2M}(t_b - t_a)\right]\right\} \\ &= \frac{1}{\sqrt{2\pi\hbar i(t_b - t_a)/M}} \sum_{l=-\infty}^{\infty} \exp\left[\frac{i}{\hbar}\frac{M}{2}\frac{(\varphi_b - \varphi_a + 2\pi l)^2}{t_b - t_a}\right]. \qquad (6.24)\end{aligned}$$

6.2 Infinite Wall

In the case of an infinite wall, only a half-space, say $x = r > 0$, is accessible to the particle, and the completeness relation reads

$$\int_0^\infty dr|r\rangle\langle r| = 1. \qquad (6.25)$$

For singular integrands, the origin has to be omitted from the integration. The orthogonality relation is

$$\langle r|r'\rangle = \delta(r - r'); \qquad r, r' > 0. \qquad (6.26)$$

Given a free particle moving in such a geometry, we want to calculate

$$(r_b t_b|r_a t_a) = \langle r_b| \prod_{n=1}^{N+1} \exp\left(-\frac{i}{\hbar}\hat{H}\epsilon\right)|r_a\rangle. \qquad (6.27)$$

As usual, we insert N completeness relations between the $N+1$ factors. In the case of a vanishing Hamiltonian, the amplitude (6.27) becomes

$$(r_bt_b|r_at_a)_0 = \prod_{n=1}^{N}\left[\int_0^\infty dr_n\right]\prod_{n=1}^{N+1}\langle r_n|r_{n-1}\rangle = \langle r_b|r_a\rangle. \tag{6.28}$$

For each scalar product $\langle r_n|r_{n-1}\rangle = \delta(r_n - r_{n-1})$, we substitute its spectral representation appropriate to the infinite-wall boundary at $r = 0$. It consists of a superposition of the free-particle wave functions vanishing at $r = 0$:

$$\begin{aligned}\langle r|r'\rangle &= 2\int_0^\infty \frac{dk}{\pi}\sin kr\sin kr' \\ &= \int_{-\infty}^\infty \frac{dk}{2\pi}\left[\exp ik(r-r') - \exp ik(r+r')\right] = \delta(r-r') - \delta(r+r').\end{aligned} \tag{6.29}$$

This Fourier representation does a bit more than what we need. In addition to the δ-function at $r = r'$, there is also a δ-function at the unphysical reflected point $r = -r'$. The reflected point plays a similar role as the periodically repeated points in the representation (6.11). For the same reason as before, we retain the reflected points in the formula as though r' were permitted to become zero or negative. Thus we rewrite the Fourier representation (6.29) as

$$\langle r|r'\rangle = \sum_{x=\pm r}\int_{-\infty}^\infty \frac{dp}{2\pi\hbar}\exp\left[\frac{i}{\hbar}p(x-x') + i\pi(\sigma(x)-\sigma(x'))\right]_{x'=r'}, \tag{6.30}$$

where

$$\sigma(x) \equiv \Theta(-x) \tag{6.31}$$

with the Heaviside function $\Theta(x)$ of Eq. (1.313). For symmetry reasons, it is convenient to liberate both the initial and final positions r and r' from their physical half-space and to introduce the localized states $|x\rangle$ whose scalar product exists on the entire x-axis:

$$\begin{aligned}\langle x|x'\rangle &= \sum_{x''=\pm x}\int_{-\infty}^\infty \frac{dp}{2\pi\hbar}\exp\left[\frac{i}{\hbar}p(x''-x') + i\pi(\sigma(x'')-\sigma(x'))\right] \\ &= \delta(x-x') - \delta(x+x').\end{aligned} \tag{6.32}$$

With these states, we write

$$\langle r|r'\rangle = \langle x|x'\rangle|_{x=r,x'=r'}. \tag{6.33}$$

We now take the trivial transition amplitude with zero Hamiltonian

$$(r_bt_b|r_at_a)_0 = \delta(r_b - r_a), \tag{6.34}$$

extend it with no harm by the reflected δ-function

$$(r_bt_b|r_at_a)_0 = \delta(r_b - r_a) - \delta(r_b + r_a), \tag{6.35}$$

and factorize it into many time slices:

$$(r_b t_b | r_a t_a)_0 = \prod_{n=1}^{N} \left[\int_0^\infty dr_n \right] \prod_{n=1}^{N+1} \left[\sum_{x_n = \pm r_n} (x_n \epsilon | x_{n-1} 0)_0 \right] \tag{6.36}$$

($r_b = r_{N+1}, r_a = r_0$), where the trivial amplitude of a single slice is

$$(x_n \epsilon | x_{n-1} 0)_0 = \langle x_n | x_{n-1} \rangle, \qquad x \in (-\infty, \infty). \tag{6.37}$$

With the help of (6.32), this can be written as

$$\begin{aligned}(r_b t_b | r_a t_a)_0 &= \prod_{n=1}^{N} \left[\int_0^\infty dr_n \right] \prod_{n=1}^{N+1} \left[\sum_{x_n = \pm r_n} \int_{-\infty}^{\infty} \frac{dp_n}{2\pi\hbar} \right] \\ &\quad \times \exp\left\{ \sum_{n=1}^{N+1} \left[\frac{i}{\hbar} p(x_n - x_{n-1}) + i\pi(\sigma(x_n) - \sigma(x_{n-1})) \right] \right\}. \end{aligned} \tag{6.38}$$

The sum over the reflected points $x_n = \pm r_n$ is now combined, at each n, with the integral $\int_0^\infty dr_n$ to form an integral over the entire x-axis, including the unphysical half-space $x < 0$. Only the last sum cannot be accommodated in this way, so that we obtain the path integral representation for the trivial amplitude

$$\begin{aligned}(r_b t_b | r_a t_a)_0 &= \sum_{x_b = \pm r_b} \prod_{n=1}^{N} \left[\int_{-\infty}^{\infty} dx_n \right] \prod_{n=1}^{N+1} \left[\int_{-\infty}^{\infty} \frac{dp_n}{2\pi\hbar} \right] \\ &\quad \times \exp\left\{ \sum_{n=1}^{N+1} \left[\frac{i}{\hbar} p(x_n - x_{n-1}) + i\pi(\sigma(x_n) - \sigma(x_{n-1})) \right] \right\}. \end{aligned} \tag{6.39}$$

The measure of this path integral is now of the conventional type, integrating over all paths which fluctuate through the entire space. The only special feature is the final symmetrization in $x_b = \pm r_b$.

It is instructive to see in which way the final symmetrization together with the phase factor $\exp[i\pi\sigma(x)] = \pm 1$ eliminates all the wrong paths in the extended space, i.e., those which cross the origin into the unphysical subspace. This is illustrated in Fig. 6.2. Note that having assumed $x_a = r_a > 0$, the initial phase $\sigma(x_a)$ can be omitted. We have kept it merely for symmetry reasons.

In the continuum limit, the exponent corresponds to an action

$$\mathcal{A}_0^\sigma[p, x] = \int_{t_a}^{t_b} dt [p\dot{x} + \hbar\pi \partial_t \sigma(x)] \equiv \mathcal{A}_0[p, x] + \mathcal{A}_{\rm topol}^\sigma. \tag{6.40}$$

The first term is the usual canonical expression in the absence of a Hamiltonian. The second term is new. It is a pure boundary term:

$$\mathcal{A}_{\rm topol}^\sigma[x] = \hbar\pi(\sigma(x_b) - \sigma(x_a)), \tag{6.41}$$

which keeps track of the topology of the half space $x > 0$ embedded in the full space $x \in (-\infty, \infty)$. This is why the action carries the subscript "topol".

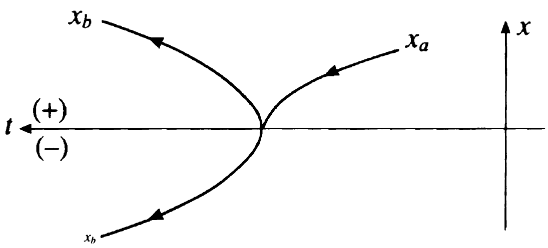


Figure 6.2 Illustration of path counting near reflecting wall. Each path touching the wall once is canceled by a corresponding path of equal action crossing the wall once into the unphysical regime (the path is mirror-reflected after the crossing). The phase factor $\exp[i\pi\sigma(x_b)]$ provides for the opposite sign in the path integral. Only paths not touching the wall at all cannot be canceled in the path integral.

The topological action (6.41) can be written formally as a local coupling of the velocity at the origin:

$$\mathcal{A}^{\sigma}_{\rm topol}[x] = -\pi\hbar \int_{t_a}^{t_b} dt\dot{x}(t)\delta(x(t)). \tag{6.42}$$

This follows directly from

$$\sigma(x_b) - \sigma(x_a) = \int_{x_a}^{x_b} dx\sigma'(x) = \int_{x_a}^{x_b} dx\Theta'(-x) = -\int_{x_a}^{x_b} dx\delta(x). \tag{6.43}$$

Consider now a free point particle in the right half-space with the usual Hamiltonian

$$H = \frac{p^2}{2M}. \tag{6.44}$$

The action reads

$$\mathcal{A}[p,x] = \int_{t_a}^{t_b} dt[p\dot{x} - p^2/2M - \hbar\pi\dot{x}(t)\delta(x(t))], \tag{6.45}$$

and the time-sliced path integral looks like (6.39), except for additional energy terms $-p_n^2/2M$ in the action. Since the new topological term is a pure boundary term, all the extended integrals in (6.39) can be evaluated right away in the same way as for a free particle in the absence of an infinite wall. The result is

$$\begin{aligned}(r_bt_b|r_at_a) \;&=\; \sum_{x_b=\pm r_b} \frac{1}{\sqrt{2\pi\hbar i(t_b-t_a)/M}} \\ &\quad\times \exp\left[\frac{i}{\hbar}\frac{M}{2}\frac{(x_b-x_a)^2}{t_b-t_a} + i\pi(\sigma(x_b)-\sigma(x_a))\right] \qquad (6.46)\\ &= \frac{1}{\sqrt{2\pi\hbar i(t_b-t_a)/M}}\left\{\exp\left[\frac{i}{\hbar}\frac{M}{2}\frac{(r_b-r_a)^2}{t_b-t_a}\right] - (r_b\to -r_b)\right\}\end{aligned}$$

with $x_a = r_a$.

This is indeed the correct result: Inserting the Fourier transform of the Gaussian (Fresnel) distribution we see that

$$\begin{aligned}(r_bt_b|r_at_a) &= \int_{-\infty}^{\infty}\frac{dp}{2\pi\hbar}\left\{\exp\left[\frac{i}{\hbar}p(r_b-r_a)\right]-(r_b\rightarrow -r_b)\right\}e^{-ip^2(t_b-t_a)/2M\hbar}\\ &= 2\int_0^{\infty}\frac{dp}{2\pi\hbar}\sin(pr_b/\hbar)\sin(pr_a/\hbar)\exp\left[-\frac{i}{\hbar}\frac{p^2}{2M}(t_b-t_a)\right],\end{aligned} \tag{6.47}$$

which is the usual spectral representation of the time evolution amplitude.

Note that the first part of (6.46) may be written more symmetrically as

$$(r_bt_b|r_at_a)=\frac{1}{\sqrt{2\pi\hbar i(t_b-t_a)/M}}\frac{1}{2}\sum_{\substack{x_a=\pm r_a\\ x_b=\pm r_b}}\exp\left[\frac{i}{\hbar}\frac{M}{2}\frac{(x_b-x_a)^2}{t_b-t_a}+i\pi(\sigma(x_b)-\sigma(x_a))\right]. \tag{6.48}$$

In this form, the phase factors $e^{i\pi\sigma(x)}$ are related to what may be considered as even and odd "spherical harmonics" in one dimension [more after (9.60)]

$$Y_{\mathrm{e},ø}(\hat{x})=\frac{1}{\sqrt{2}}(\Theta(x)\pm\Theta(-x)),$$

namely,

$$Y_{\mathrm{e}}(\hat{x})=\frac{1}{\sqrt{2}},\quad Y_{ø}(\hat{x})=\frac{1}{\sqrt{2}}e^{i\pi\sigma(x)}. \tag{6.49}$$

The amplitude (6.48) is therefore simply the odd "partial wave" of the free-particle amplitude

$$(r_bt_b|r_at_a)=\sum_{\substack{\hat{x}_b,\hat{x}_a\\ |x_b|=r_b,|x_a|=r_a}}Y_{\mathrm{o}}^{*}(\hat{x}_b)\langle x_bt_b|x_at_a\rangle Y_{ø}(\hat{x}_a), \tag{6.50}$$

which is what we would also have obtained from Schrödinger quantum mechanics.

6.3 Point Particle in Box

If a point particle is confined between two infinitely high walls in the interval $x\in(0,d)$, we speak of a *particle in a box*.[1] The box is a geometric constraint. Since the wave functions vanish at the walls, the scalar product between localized states is given by the quantum-mechanical orthogonality relation for $r\in(0,d)$:

$$\langle r|r'\rangle=\frac{2}{d}\sum_{k_\nu>0}\sin k_\nu r\sin k_\nu r', \tag{6.51}$$

[1]See W. Janke and H. Kleinert, Lett. Nuovo Cimento *25*, 297 (1979) (`http://www.physik.fu-berlin.de/~kleinert/64`).

where k_ν runs over the discrete positive momenta

$$k_\nu = \frac{\pi}{d}\nu, \quad \nu = 1, 2, 3, \ldots\ . \tag{6.52}$$

We can write the restricted sum in (6.51) also as a sum over all momenta k_ν with $\nu = 0, \pm 1, \pm 2, \ldots$:

$$\langle r|r'\rangle = \frac{1}{2d}\sum_{k_\nu}\left[e^{ik_\nu(r-r')} - e^{ik_\nu(r+r')}\right]. \tag{6.53}$$

With the help of the Poisson summation formula (6.9), the right-hand side is converted into an integral and an auxiliary sum:

$$\langle r|r'\rangle = \sum_{l=-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{dk}{2\pi}\left[e^{ik(r-r'+2dl)} - e^{ik(r+r'+2dl)}\right]. \tag{6.54}$$

Using the potential $\sigma(x)$ of (6.31), this can be re-expressed as

$$\langle r|r'\rangle = \sum_{x=\pm r}\sum_{l=-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{dk}{2\pi}e^{ik(x-x'+2dl)+i\pi(\sigma(x)-\sigma(x'))}. \tag{6.55}$$

The trivial path integral for the time evolution amplitude with a zero Hamiltonian is again obtained by combining a sequence of scalar products (6.51):

$$\begin{aligned}(r_bt_b|r_at_a)_0 &= \prod_{n=1}^{N}\left[\int_0^d dr_n\right]\langle r_n|r_{n-1}\rangle \\ &= \prod_{n=1}^{N}\left[\int_0^d dr_n\right]\prod_{n=1}^{N+1}\frac{2}{d}\sum_{k_\nu}\sin k_{\nu_n}r_n\sin k_{\nu_{n-1}}r_{n-1}.\end{aligned} \tag{6.56}$$

The alternative spectral representation (6.55) allows us to extend the restricted integrals over x_n and sums over k_ν to complete phase space integrals, and we may write

$$(r_bt_b|r_at_a)_0 = \sum_{x_b=\pm r_b}\sum_{l=-\infty}^{\infty}\prod_{n=1}^{N}\left[\int_{-\infty}^{\infty}dx_n\right]\prod_{n=1}^{N+1}\left[\int_{-\infty}^{\infty}\frac{dp_n}{2\pi\hbar}\right]\exp\left(\frac{i}{\hbar}\mathcal{A}_0^N\right), \tag{6.57}$$

with the time-sliced $H \equiv 0$ -action:

$$\mathcal{A}_0^N = \sum_{n=1}^{N+1}\left[p_n(x_n - x_{n-1}) + \hbar\pi(\sigma(x_n) - \sigma(x_{n-1}))\right]. \tag{6.58}$$

The final x_b is summed over all periodically repeated endpoints $r_b + 2dl$ and their reflections $-r_b + 2dl$.

We now add dynamics to the above path integral by introducing some Hamiltonian $H(p, x)$, so that the action reads

$$\mathcal{A} = \int_{t_a}^{t_b} dt[p\dot{x} - H(p, x) - \hbar\pi\dot{x}\delta(x)]. \tag{6.59}$$

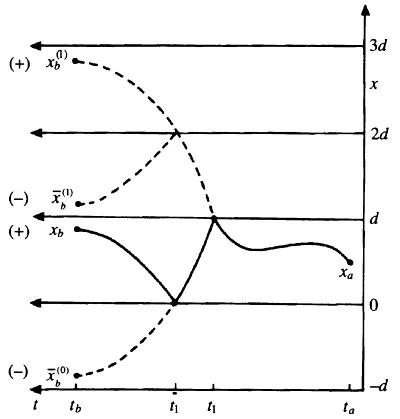


Figure 6.3 Illustration of path counting in a box. A path reflected once on the upper and once on the lower wall of the box is eliminated by a path with the same action running to $x_b^{(1)}$ and to $\bar{x}_b^{(0)}, \bar{x}_b^{(1)}$. The latter receive a negative sign in the path integral from the phase factor $\exp[i\pi\sigma(x_b)]$. Only paths remaining completely within the walls have no partner for cancellation.

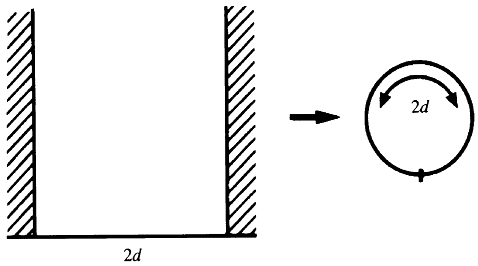


Figure 6.4 A particle in a box is topologically equivalent to a particle on a circle with an infinite wall at one point.

The amplitude is written formally as the path integral

$$(r_b t_b | r_a t_a) = \sum_{l=-\infty}^{\infty} \sum_{x_b = \pm r_b + 2dl} \int \mathcal{D}x \int \frac{\mathcal{D}p}{2\pi\hbar} \exp\left(\frac{i}{\hbar}\mathcal{A}\right). \tag{6.60}$$

In the time-sliced version, the action is

$$\mathcal{A}^N = \mathcal{A}_0^N - \epsilon \sum_{n=1}^{N+1} H(p_n, x_n). \tag{6.61}$$

The way in which the sum over the final positions $x_b = \pm r_b + 2dl$ together with the phase factor $\exp[i\pi\sigma(x_b)]$ eliminates the unphysical paths is illustrated in Fig. 6.3. The mechanism is obviously a combination of the previous two. A particle in a box of length d behaves like a particle on a circle of circumference $2d$ with a periodic boundary condition, containing an infinite wall at one point. This is illustrated in Fig. 6.4. The periodicity in $2d$ selects the momenta

$$k_\nu = (\pi/d)\nu, \quad \nu = 1, 2, 3, \ldots,$$

as it should.

For a free particle with $H = p^2/2M$, the integrations over x_n, p_n can be done as usual and we obtain the amplitude ($x_a = r_a$)

$$(r_b t_b|r_a t_a) = \sum_{l=-\infty}^{\infty} \sum_{x_b=\pm r_b+2dl} \frac{1}{\sqrt{2\pi\hbar i(t_b-t_a)/M}} \left[e^{\frac{i}{\hbar}\frac{M}{2}\frac{(x_b-x_a+2dl)^2}{t_b-t_a}} - (x_b \to -x_b) \right]. \tag{6.62}$$

A Fourier transform and an application of Poisson's formula (6.9) shows that this is, of course, equal to the quantum-mechanical expression

$$\begin{aligned}(r_b t_b|r_a t_a) &= \langle r_b|\exp\left[-\frac{i}{\hbar}(t_b-t_a)\hat{H}\right]|r_a\rangle \\ &= \frac{2}{d}\sum_{\nu=1}^{\infty} \sin k_\nu r_b \sin k_\nu r_a \exp\left[-i\hbar\frac{k_\nu^2}{2M}(t_b-t_a)\right].\end{aligned} \tag{6.63}$$

In analogy with the discussion in Section 2.6, we identify in the exponentials the eigenvalues of the energy levels labeled by $\nu - 1 = 0, 1, 2, \dots$:

$$E^{(\nu-1)} = \frac{\hbar^2 k_\nu^2}{2M}, \qquad \nu = 1, 2, 3 \dots . \tag{6.64}$$

The factors in front determine the wave functions associated with these energies:

$$\psi^{(\nu-1)}(x) = \frac{2}{d}\sin k_\nu x. \tag{6.65}$$

6.4 Strong-Coupling Theory for Particle in Box

The strong-coupling theory developed in Chapter 5 open up the possibility of treating quantum-mechanical systems with hard-wall potentials via perturbation theory. After converting divergent weak-coupling expansions into convergent strong-coupling expansions, the strong-coupling limit of a function can be evaluated from its weak-coupling expansion with any desired accuracy. Due to the combination with the variational procedure, new classes of physical systems become accessible to perturbation theory. For instance, the important problem of the pressure exerted by a stack of membranes upon enclosing walls has been solved by this method.[2]

Here we illustrate the working of that theory for the system treated in the previous section, the point particle in a one-dimensional box.

This is just a quantum-mechanical exercise for the treatment of physically more interesting problems. The ground state energy of this system has, according to Eq. (6.64), the value $E^{(0)} = \pi^2/2d^2$. For simplicity, we shall now use natural units in which we can omit Planck and Boltzmann constants everywhere, setting them equal to unity: $\hbar = 1, k_B = 1$. We shall now demonstrate how this result is found via strong-coupling theory from a perturbation expansion.

[2]See Notes and References.

6.4.1 Partition Function

The discussion becomes simplest by considering the quantum statistical partition function of the particle. It is given by the Euclidean path integral (always in natural units)

$$Z = \int \mathcal{D}u(\tau) e^{\frac{1}{2}\int_0^{\hbar\beta} d\tau (\partial u)^2}, \tag{6.66}$$

where the shifted particle coordinate $u(\tau) \equiv x(\tau) - d/2$ is restricted to the symmetric interval $-d/2 \leq u(\tau) \leq d/2$. Since such a hard-wall restriction is hard to treat analytically in (6.66), we make the hard-walls soft by adding to the Euclidean action E in the exponent of (6.66) a potential term diverging near the walls. Thus we consider the auxiliary Euclidean action

$$\mathcal{A}_{\rm e} = \frac{1}{2} \int_0^{\hbar\beta} d\tau \left\{ [\partial u(\tau)]^2 + V(u(\tau)) \right\}, \tag{6.67}$$

where $V(u)$ is given by

$$V(u) = \frac{\omega^2}{2} \left(\frac{d}{\pi} \tan \frac{\pi u}{d} \right)^2 = \frac{\omega^2}{2} \left(u^2 + \frac{2}{3} g u^4 + \dots \right). \tag{6.68}$$

On the right-hand side we have introduced a parameter $g \equiv \pi^2/d^2$.

6.4.2 Perturbation Expansion

The expansion of the potential in powers of g can now be treated perturbatively, leading to an expansion of Z around the harmonic part of the partition function. In this, the integrations over $u(\tau)$ run over the entire u-axis, and can be integrated out as described in Section 2.15. The result is [see Eq. (2.489)]

$$Z_\omega = e^{-(1/2) {\rm Tr} \log(\partial^2 + \omega^2)}. \tag{6.69}$$

For $\beta \to \infty$, the exponent gives a free energy density $F = -\beta^{-1} \log Z$ equal to the ground state energy of the harmonic oscillator

$$F_\omega = \frac{\omega}{2}. \tag{6.70}$$

The treatment of the interaction terms can be organized in powers of g, and give rise to an expansion of the free energy with the generic form

$$F = F_\omega + \omega \sum_{k=1}^{\infty} a_k \left(\frac{g}{\omega} \right)^k. \tag{6.71}$$

The calculation of the coefficients a_k in this expansion proceeds as follows. First we expand the potential in (6.67) to identify the power series for the interaction energy

$$\begin{aligned} \mathcal{A}_{\rm e}^{\rm int} &= \frac{\omega^2}{2} \int d\tau \left(g v_4 u^4 + g^2 v_6 u^6 + g^3 v_8 u^8 + \dots \right) \\ &= \frac{\omega^2}{2} \sum_{k=1}^{\infty} \int d\tau\, g^k v_{2k+2} [u^2(\tau)]^{k+1}, \end{aligned} \tag{6.72}$$

with coefficients

$$
\begin{aligned}
&v_4 = \frac{2}{3},\quad v_6 = \frac{17}{45},\quad v_8 = \frac{62}{315},\quad v_{10} = \frac{1382}{14175},\quad v_{12} = \frac{21844}{467775},\quad v_{14} = \frac{929569}{42567525},\\
&v_{16} = \frac{6404582}{638512875},\quad v_{18} = \frac{443861162}{97692469875},\quad v_{20} = \frac{18888466084}{9280784638125},\quad v_{22} = \frac{113927491862}{126109485376875},\\
&v_{24} = \frac{58870668456604}{147926426347074375},\quad v_{26} = \frac{8374643517010684}{48076088562799171875},\quad v_{28} = \frac{689005380505609448}{9086380738369043484375},\\
&v_{30} = \frac{129848163681107301953}{3952575621190533915703125},\quad v_{32} = \frac{1736640792209901647222}{122529844256906551386796875},\\
&v_{34} = \frac{418781231495293038913922}{68739242628124575327993046875},\quad \dots\,.
\end{aligned}
\tag{6.73}
$$

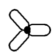
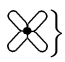
The interaction terms $\int d\tau\,[u^2(\tau)]^{k+1}$ and their products are expanded according to Wick's rule in Section 3.10 into sums of products of harmonic two-point correlation functions

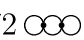
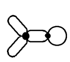
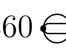
$$
\langle u(\tau_1)u(\tau_2)\rangle = \int \frac{dk}{2\pi}\,\frac{e^{ik(\tau_1-\tau_2)}}{k^2+\omega^2} = \frac{e^{-\omega|\tau_1-\tau_2|}}{2\omega}.
\tag{6.74}
$$

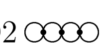
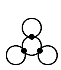
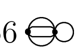
Associated local expectation values are $\langle u^2\rangle = 1/2\omega$, and

$$
\begin{aligned}
\langle u\partial u\rangle &= \int \frac{dk}{2\pi}\frac{k}{k^2+\omega^2} = 0\\
\langle \partial u\partial u\rangle &= \int \frac{dk}{2\pi}\frac{k^2}{k^2+\omega^2} = -\frac{\omega}{2},
\end{aligned}
\tag{6.75}
$$

where the last integral is calculated using dimensional regularization in which $\int dk\,k^\alpha = 0$ for all α. The Wick contractions are organized with the help of the Feynman diagrams as explained in Section 3.20. Only the connected diagrams contribute to the free energy density. The graphical expansion of free energy up to four loops is

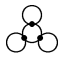
$F = \frac{\omega}{2} + \left(\frac{\omega^2}{2}\right)\Big\{ g v_4\, 3$  $+ g^2 v_6 15$  $+ g^3 v_8 105$  $\Big\}$

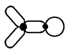
$-\frac{1}{2!}\left(\frac{\omega^2}{2}\right)^2 \Big\{ g^2 v_4^2\,[72$  $+ 24$  $] + g^3\, 2 v_4 v_6\,\big[540$  $+ 360$  $\big]\Big\}$

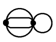
$+\frac{1}{3!}\left(\frac{\omega^2}{2}\right)^3 g^3 v_4^3 \Big\{2592$  $+ 1728$  $+ 3456$  $+ 1728$  $\Big\}.$ (6.76)

Note different numbers of loops contribute to the terms of order g^n. The calculation of the diagrams in Eq. (6.76) is simplified by the factorization property: If a diagram consists of two subdiagrams touching each other at a single vertex, the associated Feynman integral factorizes into those of the subdiagrams. In each diagram, the last t-integral yields an overall factor β, due to translational invariance along the t-axis, the others produce a factor $1/\omega$. Using the explicit expression (6.75) for the lines in the diagrams, we find the following values for the Feynman integrals:

 $= \beta\,\frac{1}{16\omega^5},$ $= \beta\,\frac{1}{64\omega^8},$

 $= \beta \dfrac{1}{32\omega^5},$  $= \beta \dfrac{3}{128\omega^8},$

 $= \beta \dfrac{1}{32\omega^6},$  $= \beta \dfrac{5}{8 \cdot 64\omega^8},$ (6.77)

 $= \beta \dfrac{1}{32\omega^6},$  $= \beta \dfrac{3}{8 \cdot 64\omega^8}.$

Adding all contributions in (6.76), we obtain up to the order g^3:

$$F_3 = \omega \left\{ \frac{1}{2} + \frac{3}{8} v_4 \left(\frac{g}{\omega} \right) + \left[\frac{15}{16} v_6 - \frac{21}{32} v_4^2 \right] \left(\frac{g}{\omega} \right)^2 + \left[\frac{105}{32} v_8 - \frac{45}{8} v_4 \, v_6 + \frac{333}{128} v_4^3 \right] \left(\frac{g}{\omega} \right)^3 \right\}, \tag{6.78}$$

which has the generic form (6.71).

We can go to higher orders by extending the Bender-Wu recursion relation (3C.20) for the ground state energy of the quartic anharmonic oscillator as follows:

$$\begin{aligned} &2p' C_n^{p'} = (p'+1)(2p'+1) C_n^{p'} + \frac{1}{2} \sum_{k=1}^{n} v_{2k+2} C_{n-k}^{p'-k-1} - \sum_{k=1}^{n-1} C_k^1 C_{n-k}^{p'}, \; 1 \leq p' \leq 2n, \\ &C_0^0 = 1, \quad C_n^{p'} = 0 \quad (n \geq 1, p' < 1). \end{aligned} \tag{6.79}$$

After solving these recursion relations, the coefficients a_k in (6.71) are given by $a_k = (-1)^{k+1} C_{k,1}$. For brevity, we list here the first sixteen expansion coefficients for F, calculated with the help of MATHEMATICA of REDUCE programs:[3]

$$\begin{aligned} &a_0 = \frac{1}{2}, \, a_1 = \frac{1}{4}, \, a_2 = \frac{1}{16}, \, a_3 = 0, \, a_4 = -\frac{1}{256}, \, a_5 = 0, \\ &a_6 = \frac{1}{2048}, \, a_7 = 0, \, a_8 = -\frac{5}{65536}, \, a_9 = 0, \\ &a_{10} = \frac{7}{524288}, \, a_{11} = 0, \, a_{12} = -\frac{21}{8388608}, \, a_{13} = 0, \\ &a_{14} = \frac{33}{67108864}, \, a_{15} = 0, \, a_{16} = -\frac{429}{4294967296}, \ldots \; . \end{aligned} \tag{6.80}$$

6.4.3 Variational Strong-Coupling Approximations

We are now ready to calculate successive strong-coupling approximations to the function $F(g)$. It will be convenient to remove the expected correct d dependence π^2/d^2 from $F(g)$, and study the function $\tilde{F}(\bar{g}) \equiv F(g)/g$ which depends only on the dimensionless reduced coupling constant $\bar{g} = g/\omega$. The limit $\omega \to 0$ corresponds to a strong-coupling limit in the reduced coupling constant $\bar{g}$. According to the general theory of variational perturbation theory and its strong-coupling limit in Sections 5.14 and 5.17, the Nth order approximation to the strong-coupling limit of $\tilde{F}(\bar{g})$, to be denoted by $\tilde{F}^*$, is found by replacing, in the series truncated after the

[3]The programs can be downloaded from www.physik.fu-berlin.de/~kleinert/b5/programs

Nth term, $\tilde{F}_N(g/\omega)$, the frequency ω by the identical expression $\sqrt{\Omega^2 - gr^2/2M}$, where

$$r^2 \equiv 2M(\Omega^2 - \omega^2)/g. \tag{6.81}$$

For a moment, this is treated as an independent variable, whereas Ω is a dummy parameter. Then the square root is expanded binomially in powers of g, and $\tilde{F}_N(g/\sqrt{\Omega^2 - gr^2/2M})$ is re-expanded up to order g^N. After that, r is replaced by its proper value. In this way we obtain a function $\tilde{F}_N(g,\Omega)$ which depends on Ω, which thus becomes a variational parameter. The best approximation is obtained by extremizing $\tilde{F}_N(g,\Omega)$ with respect to ω. Setting $\omega = 0$, we go to the strong-coupling limit $g \to \infty$. There the optimal Ω grows proportionally to g, so that $g/\Omega = c^{-1}$ is finite, and the variational expression $\tilde{F}_N(g,\Omega)$ becomes a function of $f_N(c)$. In this limit, the above re-expansion amounts simply to replacing each power ω^n in each expansion terms of $\tilde{F}_N(\bar{g})$ by the binomial expansion of $(1-1)^{-n/2}$ truncated after the $(N-n)$th term, and replacing $\bar{g}$ by c^{-1}. The first nine variational functions $f_N(c)$ are listed in Table 6.1. The functions $f_N(c)$ are minimized starting from $f_2(c)$ and searching the minimum of each successive $f_3(c)$, $f_3(c), \ldots$ nearest to the previous one. The functions $f_N(c)$ together with their minima are plotted in Fig. 6.5. The minima lie at

Table 6.1 First eight variational functions $f_N(c)$.

$$\begin{aligned}
f_2(c) &= \tfrac{1}{4} + \tfrac{1}{16\,c} + \tfrac{3\,c}{16}\\
f_3(c) &= \tfrac{1}{4} + \tfrac{3}{32\,c} + \tfrac{5\,c}{32}\\
f_4(c) &= \tfrac{1}{4} - \tfrac{1}{256\,c^3} + \tfrac{15}{128\,c} + \tfrac{35\,c}{256}\\
f_5(c) &= \tfrac{1}{4} - \tfrac{5}{512\,c^3} + \tfrac{35}{256\,c} + \tfrac{63\,c}{512}\\
f_6(c) &= \tfrac{1}{4} + \tfrac{1}{2048\,c^5} - \tfrac{35}{2048\,c^3} + \tfrac{315}{2048\,c} + \tfrac{231\,c}{2048}\\
f_7(c) &= \tfrac{1}{4} + \tfrac{7}{4096\,c^5} - \tfrac{105}{4096\,c^3} + \tfrac{693}{4096\,c} + \tfrac{429\,c}{4096}\\
f_8(c) &= \tfrac{1}{4} - \tfrac{5}{65536\,c^7} + \tfrac{63}{16384\,c^5} - \tfrac{1155}{32768\,c^3} + \tfrac{3003}{16384\,c} + \tfrac{6435\,c}{65536}\\
f_9(c) &= \tfrac{1}{4} - \tfrac{45}{131072\,c^7} + \tfrac{231}{32768\,c^5} - \tfrac{3003}{65536\,c^3} + \tfrac{6435}{32768\,c} + \tfrac{12155\,c}{131072}
\end{aligned}$$

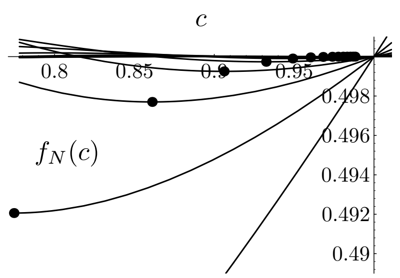


Figure 6.5 Variational functions $f_N(c)$ for particle between walls up to $N = 16$ are shown together with their minima whose y-coordinates approach rapidly the correct limiting value 1/2.

$$
\begin{aligned}
(N, f_N^{\min}) \;=\; & (2, 0.466506),\ (3, 0.492061),\ (4, 0.497701),\\
& (5, 0.499253),\ (6, 0.499738),\ (7, 0.499903),\\
& (8, 0.499963),\ (9, 0.499985), (10, 0.499994),\\
& (11, 0.499998),\ (12, 0.499999),\ (13, 0.5000),\\
& (14, 0.50000),\ (15, 0.50000),\ (16, 0.5000).
\end{aligned} \tag{6.82}
$$

They converge exponentially fast against the known result 1/2, as shown in Fig. 6.6.

6.4.4 Special Properties of Expansion

The alert reader will have noted that the expansion coefficients (6.80) possess two special properties: First, they lack the factorial growth at large orders which would be found for a single power $[u^2(\tau)]^{k+1}$ of the interaction potential, as mentioned in Eq.(3C.27) and will be proved in Eq. (17.323). The factorial growth is canceled by the specific combination of the different powers in the interaction (6.72), making the series (6.71) convergent inside a certain circle. Still, since this circle has a finite radius (the ratio test shows that it is unity), this convergent series cannot be evaluated in the limit of large g which we want to do, so that variational strong-coupling theory is not superfluous. However, there is a second remarkable property of the coefficients (6.80): They contain an infinite number of zeros in the sequence of coefficients for each odd number, except for the first one. We may take advantage of this property by separating off the irregular term $a_1 g = g/4 = \pi^2/4d^2$, setting $\alpha = g^2/4\omega^2$, and rewriting $\tilde{F}(\bar{g})$ as

$$
\tilde{F}(\alpha) = \frac{1}{4}\left[1 + \frac{1}{\sqrt{\alpha}} h(\alpha)\right], \qquad h(\alpha) \equiv \sum_{n=0}^{N} 2^{2n+1} a_{2n} \alpha^n. \tag{6.83}
$$

Inserting the numbers (6.80), the expansion of $h(\alpha)$ reads

$$
h(\alpha) = 1 + \frac{\alpha}{2} - \frac{\alpha^2}{8} + \frac{\alpha^3}{16} - \frac{5}{128}\alpha^4 + \frac{7}{256}\alpha^5 - \frac{21}{1024}\alpha^6 + \frac{33}{2048}\alpha^7 - \frac{429}{32768}\alpha^8 + \dots . \tag{6.84}
$$

We now realize that this is the binomial power series expansion of $\sqrt{1+\alpha}$. Substituting this into (6.83), we find the exact ground state energy for the Euclidean action (6.67)

$$
E^{(0)} = \frac{\pi^2}{4d^2}\left(1 + \sqrt{1 + \frac{1}{\alpha}}\right) = \frac{\pi^2}{4d^2}\left(1 + \sqrt{1 + 4\omega^2 \frac{d^4}{\pi^4}}\right). \tag{6.85}
$$

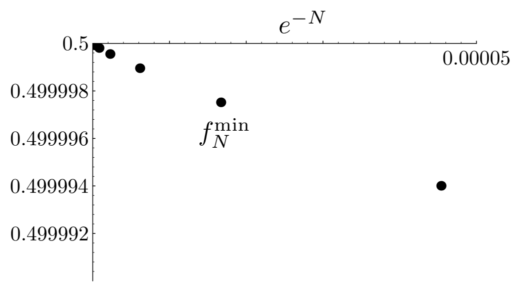


Figure 6.6 Exponentially fast convergence of strong-coupling approximations towards exact value.

Here we can go directly to the strong-coupling limit $\alpha \to \infty$ to recover the exact ground state energy $E^{(0)} = \pi^2/2d^2$.

The energy (6.85) can of course be obtained directly by solving the Schrödinger equation associated with the potential (6.72),

$$\frac{1}{2}\left\{-\frac{\partial^2}{\partial x^2} + \left[\frac{\lambda(1-\lambda)}{\cos^2 x} - 1\right]\right\}\psi(x) = \frac{d^2}{\pi^2}E\psi(x), \tag{6.86}$$

where we have replaced $u \to dx/\pi$ and set $\omega^2 d^4/\pi^4 \equiv \lambda(\lambda-1)$, so that

$$\lambda = \frac{1}{2}\left(1 + \sqrt{1 + 4\omega^2\,\frac{d^4}{\pi^4}}\right). \tag{6.87}$$

Equation (6.86) is of the Pöschl-Teller type [see Subsection 14.4.5], and has the ground state wave function, to be derived in Eq. (14.141),

$$\psi_0(x) = \text{const} \times \cos^\lambda x\,, \tag{6.88}$$

with the eigenvalue $\pi^2 E^{(0)}/d^2 = (\lambda^2 - 1)/2$, which agrees of course with Eq. (6.85).

If we were to apply the variational procedure to the series $h(\alpha)/\sqrt{\alpha}$ in F of Eq. (6.85), by replacing the factor $1/\omega^{2n}$ contained in each power α^n by $\Omega = \sqrt{\Omega^2 - r\alpha}$ and re-expanding now in powers of α rather than g, we would find that all approximation $h_N(c)$ would possess a minimum with unit value, such that the corresponding extremal functions $f_N(c)$ yield the correct final energy in *each* order N.

6.4.5 Exponentially Fast Convergence

With the exact result being known, let us calculate the exponential approach of the variational approximations observed in Fig. (6.6). Let us write the exact energy (6.85) as

$$E^{(0)} = \frac{1}{4}(g + \sqrt{g^2 + 4\omega^2}). \tag{6.89}$$

After the replacement $\omega \to \sqrt{\Omega^2 - \rho g}$, this becomes

$$E^{(0)} = \frac{\Omega}{4}\left(\hat{g} + \sqrt{\hat{g}^2 - 4\rho\hat{g} + 4}\right), \tag{6.90}$$

where $\hat{g} \equiv g/\Omega^2$. The Nth-order approximant $f_N(g)$ of $E^{(0)}$ is obtained by expanding (6.91) in powers of $\hat{g}$ up to order N,

$$f_N(g) = \Omega \sum_0^N h_k(\rho)\hat{g}^k, \tag{6.91}$$

and substituting ρ by $2Mr^2 = (1-\hat{\omega}^2)/\hat{g}$ [compare (6.81)], with $\hat{\omega}^2 \equiv \omega^2/\Omega^2$. The resulting function of $\hat{g}$ is then optimized.

It is straightforward to find an integral representation for $F_N(g)$. Setting $r\hat{g} \equiv z$, we have

$$F_N = \frac{1}{2\pi i}\oint_{C_0} \frac{dz}{z^{N+1}}\frac{1 - z^{N+1}}{1-z}\,f(z), \tag{6.92}$$

where the contour C_0 refers to small circle around the origin and

$$\begin{aligned} F(z) &= \frac{\Omega}{4}\left(\frac{z}{r} + \sqrt{\frac{z^2}{r^2} - 4z + 4}\right) \\ &= \frac{1}{4r}\left(z + \sqrt{(z-z_1)(z-z_2)}\right), \end{aligned} \tag{6.93}$$

with branch points at $z_{1,2} = 2r^2\left(1 \pm \sqrt{1-1/r^2}\right)$. For $z < 1$, we rewrite

$$
\begin{aligned}
&1 - z^{N+1} = (1-z)(1+z+\ldots+z^N) = (1-z)(N+1)\\
&-(1-z)^2\left[N+(N-1)z+\ldots+z^{N-1}\right]
\end{aligned}
\tag{6.94}
$$

and estimate this for $z \approx 1$ as

$$
1 - z^{N+1} = (1-z)(N+1) + \mathcal{O}(|1-z|^2\, N^2). \tag{6.95}
$$

Dividing the approximant (6.92) by Ω, and indicating this by a hat, we use (6.94) to write $\hat{F}_N$ as a sum over the discontinuities across the two branch cuts:

$$
\begin{aligned}
\hat{F}_N &= \frac{(N+1)}{2\pi i}\oint_{C_0}\frac{dz\hat{F}(z)}{z^{N+1}}\hat{F}(z) = \frac{(N+1)}{N!}\hat{F}^{(N)}(0)\\
&= (N+1)\sum_{i=1}^{2}\int_{z_i}^{\infty}\frac{dz}{z^{N+1}}\hat{F}(z).
\end{aligned}
\tag{6.96}
$$

The integrals yield a constant plus a product

$$
\Delta\hat{F}_N \approx \frac{(N+1)(N-\frac{3}{2})!}{N!}\frac{1}{(r^2)^N}\frac{1}{(1+r^2)^N}, \tag{6.97}
$$

which for large N can be approximated using Stirling's formula (5.204) by

$$
\Delta\hat{F}_N \approx \frac{A}{(r^2)^N\sqrt{N}}e^{-r^2N}. \tag{6.98}
$$

In the strong-coupling limit of interest here, $\hat{\omega}^2 = 0$, and $r = 1/\hat{g} = \Omega/g = c$. In Fig. 6.5 we see that the optimal c-values tend to unity for $N \to \infty$, so that $\Delta\hat{f}_N$ goes to zero like e^{-N}, as observed in Fig. 6.6.

Notes and References

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