CHAPTER V

SYSTEMATIC IMPROVING FEYNMAN VARIATIONAL APPROACH

Functional in Fourier Space

At this point we introduce a technical observation concerning statistical path integrals. Instead of the zigzag formulation of paths on a sliced time axis, we use the Fourier decomposition of paths on the continuous time axis by expanding these paths as follows [Feynman and Hibbs 1965, Kleinert 1990]

$$x(\tau) \;=\; x_0 + \sum_{m=1}^{\infty} \left(x_m e^{\,i\omega_m \tau} + c.c.\right), \qquad x_0 = \text{real}\,. \tag{5.1}$$

For this case the sum is unrestricted and run over all Matsubara frequencies $\omega_m = 2\pi m / \beta\hbar$ with $\beta = 1/k_B T$. In terms of these x_m's the euclidean action of the harmonic oscillator is

$$\begin{aligned} S \;&=\; \int_0^{\beta\hbar} d\tau \left(\frac{M}{2}\dot{x}^{\,2} + \frac{M}{2}\omega^2 x^2\right) \\ &=\; M\beta\hbar \left[\frac{\omega^2}{2} x_0^2 + \sum_{m=1}^{\infty} \left(\omega_m^2 + \omega^2\right) |x_m|^2\right]. \end{aligned} \tag{5.2}$$

We now see that the result (3.71) can also be obtained by using this decomposition of S together with the following measure of integration

$$\int \mathcal{D}x \;\equiv\; \int_{-\infty}^{\infty} \frac{dx_0}{\sqrt{2\pi\beta\hbar^2/M}} \prod_{m=1}^{\infty} \left[\int_{-\infty}^{\infty} \frac{dx_m^{re}\, dx_m^{im}}{\pi/\beta M\omega_m^2}\right], \tag{5.3}$$

where the short notation $x_m^{re} = \text{Re}\, x_m$ and $x_m^{im} = \text{Im}\, x_m$. We can make use of the measure in above by showing, in the high temperature limit, the path integral representation of any quantum partition function reduces to the classical partition function. We start out with the Lagrangian formulation (3.37) and inserting the Fourier decomposition (5.1). Then, the kinetic term becomes

$$\int_0^{\beta\hbar} \frac{M}{2}\dot{x}^2 = M\beta\hbar \sum_{m=1}^{\infty} \omega_m^2 |x_m|^2 \tag{5.4}$$

and the partition function can be expressed as

$$Z = \int \mathcal{D}x \exp\left\{ -\beta M \sum_{m=1}^{\infty} \omega_m^2 |x_m|^2 \right.$$
$$\left. -\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau\, V\left(x_0 + \sum_{m=-\infty}^{\infty}{}' x_m e^{i\omega_m \tau} \right)\right\}, \tag{5.5}$$

where a prime symbol means the absence of the $m = 0$ mode. We now observe that, for large temperature, the Matsubara frequencies for $m \neq 0$ diverge like $2\pi m / \beta\hbar$. This has that the Boltzmann factor for the fluctuations becomes sharply around x_0. The average size of x_m is $\sqrt{1/\beta M} / \omega_m = \hbar / 2\pi m \sqrt{M/\beta}$. If the potential is smooth in its arguments, we can approximate it by $V(x_0)$ plus powers of x_m. For large temperature these are small on the average and can be ignored. The leading term $V(x_0)$ is time dependent and then, in the high temperature limit, we obtain

$$Z \xrightarrow{T \to \infty} \int \mathcal{D}x \exp\left\{ \beta M \sum_{m=1}^{\infty} \omega_m^2 |x_m|^2 - \beta V(x_0) \right\}. \tag{5.6}$$

The right-hand side is quadratic in the component x_m. Thus, if we use the measure (5.3), we can do the integrals over x_m and obtain

$$Z \xrightarrow{T \to \infty} Z_{cl} = \int_{-\infty}^{\infty} \frac{dx_0}{\sqrt{2\pi\beta\hbar^2 / M}} e^{-\beta V(x_0)} \tag{5.7}$$

This also agree with the classical partition function (3.19). Notice that the zero component is

$$x_0 = \frac{1}{\beta\hbar}\int_0^{\beta\hbar} x(\tau)\, d\tau \tag{5.8}$$

which is the average position of any path discussed before in previous chapter.

The Effective Classical Potential

We now consider the path integral of a point particle moving in one dimensional potential $V(x(\tau))$. The path integral representation of a quantum mechanical partition function

$$Z \equiv e^{-\beta F} \equiv \int \mathcal{D}x(\tau) \exp\left\{-\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau \left(\frac{M}{2}\dot{x}^2(\tau) + V(x(\tau))\right)\right\} \tag{5.9}$$

involves an infinite product of ordinary integrals. After a Fourier decomposition of the periodic paths as described in before the integration measure has been expressed in term of the Fourier components

$$Z = \int_{-\infty}^{\infty} \frac{dx_0}{\sqrt{2\pi\beta\hbar^2 / M}} \prod_{m=1}^{\infty} \left[\int \frac{dx_m^{re}\, dx_m^{im}}{\pi / \beta M \omega_m^2}\right]$$

$$\times \exp\left\{-\beta M \sum_{m=1}^{\infty} \omega_m^2 |x_m|^2 - \frac{1}{\hbar}\int_0^{\beta\hbar} d\tau\, V\left(x_0 + \left(\sum_{m=1}^{\infty} x_m e^{i\omega_m \tau} + c.c.\right)\right)\right\}. \tag{5.10}$$

we imagine that we could succeed in integrating out all real and imaginary components of x_m with $m \neq 0$. This would leave Z as a simple integral over the remaining zero frequency component x_0. Then we can write

$$Z = \int_{-\infty}^{\infty} \frac{dx_0}{\sqrt{2\pi\beta\hbar^2 / M}} e^{-\beta V_{eff,cl}(x_0)} , \qquad (5.11)$$

where in high temperature limit we can do so. The potential $V_{eff,cl}(x_0)$ is some function of x_0, which is the average position of the fluctuating path on the time interval $[0, \beta\hbar]$. The remaining integral (5.11) has the same form as a classical partition function expressed before in (5.7),

$$Z_{cl} = \int_{-\infty}^{\infty} \frac{dx_0}{\sqrt{2\pi\beta\hbar^2 / M}} e^{-\beta V(x_0)} , \qquad (5.12)$$

resulting in the classical limit $V_{eff,cl} \rightarrow V(x_0)$ as $T \rightarrow \infty$. This is why the function $V_{eff,cl}(x_0)$ is referred to as the *effective classical potential* and to the integral (5.11) as the *effective classical partition function.* It accounts for the effects of all quantum fluctuations [Feynman and Hibbs 1965, Feynman 1972].

It is interesting to see what this potential looks like in the case of a harmonic oscillator where it can be calculated exactly. Then the Boltzmann factor in (5.11) is simply

$$\exp\left\{ -\beta M \sum_{n=1}^{\infty} (\omega_m^2 + \omega^2) | x_m |^2 \right\} e^{-\beta M \omega^2 x_0^2/2} . \qquad (5.13)$$

The integrals over x_m^{re} x_m^{im} can be performed with the result

$$Z = \int_{-\infty}^{\infty} \frac{dx_0}{\sqrt{2\pi\beta\hbar^2 / M}} \prod_{m=1}^{\infty} \left[\frac{\omega_m^2}{\omega_m^2 + \omega^2} \right] e^{-\beta M \omega^2 x_0{}^2/2} . \qquad (5.14)$$

The remaining Boltzmann factor contains the potential energy at the average path position x_0 only. The accompanying product over the frequency ratios was evaluated before in (3.70),

$$\prod_{m=1}^{\infty} \frac{\omega_m^2}{\omega_m^2 + \omega^2} = \frac{\beta\hbar\omega/2}{\sinh\left(\beta\hbar\omega/2\right)}. \qquad (5.15)$$

Hence we find the full quantum partition function as the single integral of the form (5.11), with the effective classical potential

$$\begin{aligned} V_{eff,\,cl}(x_0) &= \frac{1}{\beta}\log\frac{\sinh\left(\beta\hbar\omega/2\right)}{\beta\hbar\omega/2} + V(x_0) \\ &= -\frac{1}{\beta}\log\beta\hbar\omega + \frac{\hbar\omega}{2} + \frac{1}{\beta}\log\left(1 - e^{-\beta\hbar\omega}\right) + V(x_0). \qquad (5.16) \end{aligned}$$

Thus, in the case of the harmonic oscillator, the effective classical potential is simply changed which respect to the classical potential at the average path position x_0 by an additional temperature dependent constant. In the limit of small temperature we have,

$$V_{eff,\,cl}(x_0) \xrightarrow{T \to 0} \frac{\hbar\omega}{2} + V(x_0), \qquad (5.17)$$

i.e., the additional constant tends to $\hbar\omega/2$. This is just the quantum mechanical zero-point energy. It guarantees that the partition function (5.13) has the correct zero-temperature quantum limit

$$\begin{aligned} Z &\xrightarrow{T \to 0} e^{-\beta\hbar\omega/2}\,\beta\hbar\omega \int_{-\infty}^{\infty} \frac{dx_0}{\sqrt{2\pi\beta\hbar^2/M}}\, e^{-\beta M\omega^2 x_0^2/2} \\ &= e^{-\beta\hbar\omega/2}, \qquad (5.18) \end{aligned}$$

with the zero-point oscillations in $1/T$.

Feynman-Kleinert Variational Approach

For a general quantum mechanical system with any potential $V(x)$ it is impossible to calculate $V_{eff,\,cl}(x_0)$ exactly. We, however, try to find a simple but very accurate approximation to $V_{eff,\,cl}(x_0)$ which, moreover, approaches the true $V_{eff,\,cl}(x_0)$ from above. It is obtained by comparing the path integral in question with a soluble trial path integral which is a suitable superposition of harmonic oscillator path integrals centered at various average positions x_0, each of them having its own x_0-dependent frequency $\Omega(x_0)$. At the end, the superposition and the frequency will be chosen optimally in such a way that the effective classical potential of the trial system is an upper bound to the unknown one.

The trial potential of the potential $V_{eff,\,cl}(x_0)$ is designed for the trial action S_1 as follow [Feynman and Kleinert 1986]

$$S_1 \;=\; \int_0^{\beta\hbar} d\tau \left[\frac{M}{2}\dot{x}^{\,2} + \frac{M}{2}\Omega^{2}(x_0)\,(x - x_0)^2 + L_1(x_0)\right]. \qquad (5.19)$$

Thus, the partition function to be used is given by

$$Z_1 \;\equiv\; e^{-\beta F_1} \;=\; \int \mathcal{D}x(\tau)$$

$$\times \exp\left\{-(1/\hbar)\int_0^{\beta\hbar} d\tau\, \frac{M}{2}\left[\dot{x}^{\,2} + \Omega^{2}(x_0)\,(x - x_0)^2\right]\right\} e^{-\beta L_1(x_0)}. \qquad (5.20)$$

It involves two unknown x_0-dependent functions, the superposition function $L_1(x_0)$ and the frequency $\Omega(x_0)$, where F_1 is defined as the free energy corresponding to this trial partition function. Expanding the kinetic term into its Fourier components, it contributes to the exponent a term

$$- \beta M \sum_{m=1}^{\infty} \left(\omega_m^2 + \Omega^2(x_0)\right) | x_m |^2 . \tag{5.21}$$

We can then perform the integrals over x_m^{re} , x_m^{im} just as in the case of a harmonic oscillator in the previous example, Eq. (5.13), and obtain

$$Z_1 = \int_{-\infty}^{\infty} \frac{dx_0}{\sqrt{2\pi\beta\hbar^2 / M}} \frac{\beta\hbar\Omega(x_0)/2}{\sinh\left(\beta\hbar\Omega(x_0)/2\right)} e^{-\beta L_1(x_0)} . \tag{5.22}$$

This may be rewritten as a classical partition function

$$Z_1 = \int_{-\infty}^{\infty} \frac{dx_0}{\sqrt{2\pi\beta\hbar^2 / M}} e^{-\beta W_1(x_0)} , \tag{5.23}$$

with an approximate effective classical potential

$$W_1(x_0) \equiv \frac{1}{\beta} \ln \frac{\sinh\left(\beta\hbar\Omega(x_0)/2\right)}{\beta\hbar\Omega(x_0)/2} + L_1(x_0) . \tag{5.24}$$

We would like to determine the two trial functions $\Omega^2(x_0)$ and $L_1(x_0)$ in such a way that $W_1(x_0)$ becomes an optimal upper bound and thus a very good approximation to the effective classical partition function $V_{eff,\,cl}(x_0)$ over a wide range of temperatures.

To solve this problem we take recourse in an extremal principle. We shall first find an inequality for the trial function $\Omega^2(x_0)$ and $L_1(x_0)$ ensuring that Z_1 is always smaller than Z and select those functions which make Z_1 largest. For the corresponding free energies F_1 and F this will supply an optimal upper bound F_1 for F. Afterwards we shall extend the inequality by proving that it holds also locally in the form $W_1(x_0) \geq V_{eff,\,cl}$. It will turn out that for many potentials $V(x)$, this procedure will bring F_1 so close to F that the difference is only a few percent, even at zero temperature where the effect of quantum fluctuations is most relevant.

To find the optimal bound we are based on the Jensen - Peierls inequality and the variational approach as fundamentally described before in Chapter IV We rewrite the original partition function as follows

$$Z = \int \mathcal{D}x e^{-(1/\hbar)S}$$

$$= \int \mathcal{D}x e^{-(1/\hbar)S_1} e^{-(1/\hbar)(S - S_1)}, \tag{5.25}$$

where S_1 is the trial euclidean action (5.19) of the trial partition function (5.20) whose path integral was reduced to the single integral (5.23). The second expression for Z may further be rewritten as

$$Z = Z_1 \langle e^{-(1/\hbar)(S - S_1)} \rangle_1 , \tag{5.26}$$

where the bracket $\langle \cdot \cdot \cdot \rangle_1$ denote the expectation value calculated with the trial probability distribution $\exp\{-S_1/\hbar\}$. More precisely, for an arbitrary functional $\mathcal{O}[x]$ of the path $x(\tau)$ we define

$$\langle \mathcal{O}[x] \rangle_1 = Z_1^{-1} \int \mathcal{D}x e^{-(1/\hbar)S_1} \mathcal{O}[x] . \tag{5.27}$$

we now observe that, for any probability distribution, the expectation of an exponential is always larger than the exponential of an expectation:

$$\langle e^{\mathcal{O}} \rangle \geq e^{\langle \mathcal{O} \rangle} . \tag{5.28}$$

This inequality, Jensen - Peierls inequality, can therefore be used to write down immediately an inequality for the partition function Z in (5.26),

$$Z \geq Z_1 e^{-(1/\hbar)\langle S - S_1 \rangle_1} . \tag{5.29}$$

for the free energies $F = -(1/\beta)\ln Z$, this implies the upper bound

$$F \;\leq\; F_1 + \frac{1}{\beta\hbar}\langle S - S_1\rangle_1 \,. \tag{5.30}$$

Since the two actions S and S_1 have the same kinetic term $\int d\tau (M/2)\dot{x}^2$ (this is how S_1 was constructed), only the potential terms survive in the difference and we remain with

$$F \;\leq\; F_1 + \frac{1}{\beta\hbar}\int_0^{\beta\hbar} d\tau \left\langle V(x(\tau)) - \frac{M}{2}\Omega^2(x_0)\left(x(\tau) - x_0\right)^2 - L_1(x_0)\right\rangle_1 . \tag{5.31}$$

On the right-hand side we must calculate the expectation of the potentials $V(x(\tau))$ and of the trial potential $L_1(x_0)$ within the measure of the partition function Z_1. Let us start with $V(x(\tau))$. For this we decompose $V(x(\tau))$ into its Fourier components

$$V(x(\tau)) \;=\; \int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{\,ikx(\tau)}\, \tilde{V}(k) \,. \tag{5.32}$$

Using the partition function Z_1 in the form (5.10) and (5.27), the expectation is written as follows,

$$\begin{aligned}\langle V(x(\tau))\rangle_1 \;=\; & Z_1^{-1}\int_{-\infty}^{\infty} \frac{dx_0}{\sqrt{2\pi\beta\hbar^2/M}} \prod_{m=1}^{\infty}\left[\int \frac{dx_m^{re}\, dx_m^{im}}{\sqrt{\pi/\beta M\omega_m^2}}\right] \\ & \times \exp\left\{ -\beta M \sum_{m=1}^{\infty} \left(\omega_m^2 + \Omega^2(x_0)\right)|x_m|^2 - \beta L_1(x_0)\right\} \\ & \times \int_{-\infty}^{\infty} \frac{dk}{2\pi} \tilde{V}(k)\, e^{\,ik\left[x_0 + \sum_{m=1}^{\infty}\left(x_m e^{i\omega_m \tau} + c.c.\right)\right]} \,. \end{aligned} \tag{5.33}$$

As far as the x_m-integrals are concerned, the only new term with respect to the partition function Z_1 itself is the exponent $\exp\left\{ ik\,\Sigma_{m=1}^{\infty} x_m\, e^{i\omega_m \tau} + c.c.\right\}$. This can be combined with the exponent of the kinetic term by a quadratic completion, giving

$$\exp\left\{ -\beta M \sum_{m=1}^{\infty} \left(\omega_m^2 + \Omega^2(x_0)\right)\left[\left(x_m^{re} - ik\frac{1/\beta M}{\omega_m^2 + \Omega^2(x_0)}\cos\omega_m\tau\right)^2 \right.\right.$$
$$\left.\left. + \left(x_m^{im} - ik\frac{1/\beta M}{\omega_m^2 + \Omega^2(x_0)}\sin\omega_m\tau\right)^2\right] - \frac{a^2(x_0)}{2}k^2\right\} \tag{5.34}$$

where $a^2(x_0)$ is the sum

$$a^2(x_0) = \frac{2}{\beta M}\sum_{m=1}^{\infty}\frac{1}{\omega_m^2 + \Omega^2(x_0)}. \tag{5.35}$$

It has the dimension of a square length. The Gaussian integrals over x_m^{re}, x_m^{im} can now be done just as in Z_1 itself and we remain with

$$\langle V(x(\tau))\rangle_1 = Z_1^{-1}\int_{-\infty}^{\infty}\frac{dx_0}{\sqrt{2\pi\beta\hbar^2/M}}\frac{\beta\hbar\Omega(x_0)/2}{\sinh\left(\beta\hbar\Omega(x_0)/2\right)}$$
$$\times\int_{-\infty}^{\infty}\frac{dk}{2\pi}\tilde{V}(k)e^{ikx_0 - a^2(x_0)k^2/2} \tag{5.36}$$

Notice that the τ-dependence in $x(\tau)$ has disappeared. Inserting the Fourier representation of $\tilde{V}(k)$.

$$\tilde{V}(k) = \int_{-\infty}^{\infty} dx\, V(x)\, e^{-ikx}, \tag{5.37}$$

we can perform the k integral, again via quadratic completion, and the last factor in (5.36) becomes

$$V_{a^2(x_0)}(x_0) \equiv \int_{-\infty}^{\infty} \frac{dx_0'}{\sqrt{2\pi a^2(x_0)}} e^{-(x_0'-x_0)^2/2a^2(x_0)} V(x_0') . \tag{5.38}$$

Thus $V_{a^2}(x_0)$ arises from the original potential by smearing it out in the neighbourhood of each point x_0 with a Gaussian distribution of width $a(x_0)$. This smearing accounts for the quantum statistical fluctuations. In terms of $V_{a^2}(x_0)$ we find

$$\langle V(x(\tau))\rangle_1 = Z_1^{-1} \int_{-\infty}^{\infty} \frac{dx_0}{\sqrt{2\pi\beta\hbar^2/M}} \frac{\beta\hbar\Omega(x_0)/2}{\sinh\left(\beta\hbar\Omega(x_0)/2\right)}$$

$$\times V_{a^2(x_0)}(x_0)\, e^{-\beta L_1(x_0)} , \tag{5.39}$$

which is the first expectation in (5.31).

It is now also quite easy to calculate also the second expectation in (5.31), namely $\left\langle \left(\Omega^2(x_0)/2\right)(x(\tau)-x_0)^2\right\rangle_1$. First we write down the smeared out version of $(x-x_0)^2$,

$$(x-x_0)^2_{a^2} = \int_{-\infty}^{\infty} \frac{dx'}{\sqrt{2\pi a^2}} e^{-(1/2a^2)(x'-x)^2} (x'-x_0)^2 =$$

$$\int_{-\infty}^{\infty} \frac{dx'}{\sqrt{2\pi a^2}} e^{-(1/2a^2)(x'-x)^2} \left[(x'-x)^2 + 2(x-x_0)(x'-x) + (x-x_0)^2\right] . \tag{5.40}$$

Using the Gaussian integrals

$$\int_{-\infty}^{\infty} \frac{dx'}{\sqrt{2\pi a^2}} e^{-(1/2a^2)(x'-x)^2} (x'-x)^n = \begin{Bmatrix} n!!a^n \\ 0 \end{Bmatrix} \text{ for } n = \begin{Bmatrix} \text{even} \\ \text{odd} \end{Bmatrix}, \tag{5.41}$$

we have

$$(x-x_0)^2_{a^2} = (x-x_0)^2 + a^2 . \tag{5.42}$$

According to (5.39), the expectation $\langle (x(\tau) - x_0)^2 \rangle_1$ is an integral over the corresponding $V_{a^2(x_0)}(x_0)$ which in this case requires forming the smeared potential $(x - x_0)^2_{a^2(x_0)}$ and inserting $x = x_0$ into it. But for $x = x_0$ the first term in (5.42) vanishes and only $a(x_0)^2$ survives.

The expectation in (5.31) reduces therefore to the τ-independent single integral

$$\left\langle V(x(\tau)) - \frac{M}{2}\Omega^2(x_0)(x(\tau) - x_0)^2 - L_1(x_0)\right\rangle_1$$

$$= Z_1^{-1}\int_{-\infty}^{\infty}\frac{dx_0}{\sqrt{2\pi\beta\hbar^2/M}}\frac{\beta\hbar\Omega(x_0)/2}{\sinh\left(\beta\hbar\Omega(x_0)/2\right)}$$

$$\times\left[V_{a^2}(x_0) - \frac{M}{2}\Omega^2(x_0)a^2(x_0) - L_1(x_0)\right]e^{-\beta L_1(x_0)}, \qquad (5.43)$$

It is independent of τ so that we may write the inequality (5.31) as

$$F \leq F_1 + \left\langle V_{a^2}(x_0) - \frac{M}{2}\Omega^2(x_0)a^2(x_0) - L_1(x_0)\right\rangle_1, \qquad (5.44)$$

with the expectation $\langle\ldots\rangle_1$ being the single integral (5.43).

<u>**Optimizing the Trial Partition Function**</u>

We now choose the trial function $L_1(x_0)$ to minimize the right-hand side of (5.44). Varying $L_1(x_0) \to L_1(x_0) + \delta L_1(x_0)$ we find

$$\delta Z_1 = -\beta Z_1 \langle \delta L_1(x_0)\rangle_1, \qquad (5.45)$$

and hence

$$\delta F_1 = \langle \delta L_1(x_0)\rangle_1. \qquad (5.46)$$

Furthermore,

$$\delta\left\langle V_{a^2}(x_0) - \frac{M}{2}\Omega^2(x_0)a^2(x_0) - L_1(x_0)\right\rangle_1$$

$$= \delta\left\{Z_1^{-1}\int_{-\infty}^{\infty}\frac{dx_0}{\sqrt{2\pi\beta\hbar^2/M}}\frac{\beta\hbar\Omega(x_0)/2}{\sinh\left(\beta\hbar\Omega(x_0)/2\right)}\right.$$

$$\left.\times\left[V_{a^2}(x_0) - \frac{M}{2}\Omega^2(x_0)a^2(x_0) - L_1(x_0)\right]e^{-\beta L_1(x_0)}\right\}$$

$$= \beta\left\{\left\langle\delta L_1(x_0)\right\rangle_1\left\langle V_{a^2}(x_0) - \frac{M}{2}\Omega^2(x_0)a^2(x_0) - L_1(x_0)\right\rangle_1\right.$$

$$\left.-\,\delta L_1(x_0)\times\left\langle\left[V_{a^2}(x_0) - \frac{M}{2}\Omega^2(x_0)a^2(x_0) - L_1(x_0)\right]\right\rangle_1\right\} - \left\langle\delta L_1(x_0)\right\rangle_1 . \qquad (5.47)$$

This shows that the right-hand side of (5.38) is extremal if we choose

$$L_1(x_0) \;=\; V_{a^2}(x_0) - \frac{M}{2}\Omega^2(x_0)a^2(x_0) . \qquad (5.48)$$

The second derivative proves this to be a minimum. Then F is bounded directly by F_1 from above,

$$F \leq F_1 , \qquad (5.49)$$

with F_1 given by

$$F_1 = -\frac{1}{\beta}\ln Z_1 = -\frac{1}{\beta}\ln\int_{-\infty}^{\infty}\frac{dx_0}{\sqrt{2\pi\beta\hbar^2/M}}e^{-\beta W_1(x_0)} , \qquad (5.50)$$

where the potential $W_1(x_0)$ is given by

$$W_1(x_0) \equiv \frac{1}{\beta}\ln\frac{\sinh\beta\hbar\Omega(x_0)/2}{\beta\hbar\Omega(x_0)/2} + V_{a^2}(x_0) - \frac{M}{2}\Omega^2(x_0)a^2(x_0) . \qquad (5.51)$$

Having obtained this result one may suspect that the inequality $F \leq F_1$, when written in the form

$$\int_{-\infty}^{\infty} \frac{dx_0}{\sqrt{2\pi\beta\hbar^2 / M}} e^{-\beta V_{eff,cl}(x_0)} \geq \int_{-\infty}^{\infty} \frac{dx_0}{\sqrt{2\pi\beta\hbar^2 / M}} e^{-\beta W_1(x_0)} \qquad (5.52)$$

holds also locally at each point x_0, i.e.,

$$e^{-\beta V_{eff,cl}(x_0)} \geq e^{-\beta W_1(x_0)} . \qquad (5.53)$$

Indeed, this can easily be shown by invoking the Jensen-Peierls inequality at each fixed x_0, using a slight modification of the measure in which only the x_m's with $m \neq 0$ are integrated. In other words, the relations (5.25) - (5.30) are all satisfied with the measure $\int \mathcal{D}x(\tau)\delta(x_0 - \bar{x}_0)$ at a fixed path average $\bar{x}_0$. In such a local derivation the trial function $L_1(x_0)$ disappears identically.

We are now ready to determine the unknown trial function $\Omega^2(x_0)$ by minimizing $W_1(x_0)$. The partial derivative of $W_1(x_0)$ with respect to $\Omega^2(x_0)$ has two terms

$$\frac{dW_1(x_0)}{d\Omega^2(x_0)} = \frac{\partial W_1(x_0)}{\partial\Omega^2(x_0)} + \left.\frac{\partial W_1(x_0)}{\partial a^2(x_0)}\right|_{\Omega(x_0)} \frac{\partial a^2(x_0)}{\partial\Omega^2(x_0)} . \qquad (5.54)$$

The first term is equal to

$$\frac{\partial W_1(x_0)}{\partial\Omega^2(x_0)} = \frac{M}{2}\left\{\frac{\beta}{M\Omega^2(x_0)}\left[\frac{\beta\hbar\Omega}{2}\coth\left(\frac{\beta\hbar\Omega}{2}\right) - 1\right] - a^2(x_0)\right\} \qquad (5.55)$$

and happens to vanish automatically due to (5.35). Indeed, the sum there is easily calculated as follows

$$\begin{aligned} a^2(x_0) &= \frac{2}{\beta M}\frac{\partial}{\partial\Omega^2}\ln\prod_{m=1}^{\infty}\frac{\omega_m^2 + \Omega^2(x_0)}{\omega_m^2} \\ &= \frac{1}{\beta M}\frac{1}{\Omega}\frac{\partial}{\partial\Omega}\ln\frac{\sinh\left(\beta\hbar\Omega(x_0)/2\right)}{\beta\hbar\Omega(x_0)/2} \end{aligned}$$

$$= \frac{1}{\beta M\Omega^2(x_0)}\left(\frac{\beta\hbar\Omega(x_0)}{2}\coth\frac{\beta\hbar\Omega(x_0)}{2} - 1\right). \tag{5.56}$$

Thus we merely have to find the minimum of $W_1(x_0)$ with respect to $a^2(x_0)$, i.e.,

$$\frac{\partial W_1}{\partial a^2} = 0. \tag{5.57}$$

With (5.51), this gives the relation

$$\Omega^2(x_0) = \frac{2}{M}\frac{\partial V_{a^2(x_0)}(x_0)}{\partial a^2(x_0)}. \tag{5.58}$$

Moreover, since $V_{a^2}(x_0)$ is given by

$$\int_{-\infty}^{\infty}\frac{dk}{2\pi}e^{-(a^2/2)k^2}\tilde{V}(k)e^{ikx_0}, \tag{5.59}$$

the derivative $2\left(\partial/\partial a^2\right)V_{a^2}$ amounts to a factor $-k^2$ inside the Fourier representation, so that we can also write

$$\Omega^2(x_0) = \frac{1}{M}\left[\frac{\partial^2}{\partial x_0^2}V_{a^2}(x_0)\right]_{a^2=a^2(x_0)}. \tag{5.60}$$

Note that the partial derivatives is performed at fixed a^2 which is set equal to $a^2(x_0)$ at the end.

The potential $W_1(x_0)$ with this optimal choice of $\Omega^2(x_0)$ and $a^2(x_0)$ determined from (5.56) represents the Feynman-Kleinert approximation to the effective classical potential $V_{eff,\,cl}(x_0)$ which we wanted to calculate.

Notice that since (5.56) makes

$$\frac{\partial W_1(x_0)}{\partial\Omega^2(x_0)} = 0, \tag{5.61}$$

it is possible to consider both functions $\Omega^2(x_0)$ and $a^2(x_0)$ as arbitrary trial functions in $W_1(x_0)$ of Eq. (5.51) to be determined by independent. The author introduced an alternative way of choosing Ω as (5.60), see the Appendix.

Application to Anharmonic Oscillator

At this point we consider the anharmonic oscillator as the first application due to the Feynman-Kleinert variational approach. Consider the anharmonic oscillator under the potential

$$V(x) = \frac{1}{2}x^2 + \frac{1}{4}gx^4, \tag{5.62}$$

where g is the positive coupling constant. The euclidean action of this system is written as

$$S = \int_0^{\beta\hbar} d\tau\left(\frac{M}{2}\dot{x}^2 + \frac{1}{2}x^2 + \frac{1}{4}gx^4\right). \tag{5.63}$$

The smeared potential obey the expression (5.38) is

$$\begin{aligned} V_{a^2}(x_0) &= \int_{-\infty}^{\infty} \frac{dx'}{\sqrt{2\pi a^2}} e^{-(1/2a^2)(x'-x_0)^2}\left(\frac{1}{2}x'^2 + \frac{1}{4}gx'^4\right) \\ &= \int_{-\infty}^{\infty} \frac{dx'}{\sqrt{2\pi a^2}} e^{-(1/2a^2)(x'-x_0)^2}\left\{\frac{x^2}{2} + x(x'-x_0) + \frac{(x'-x_0)^2}{2}\right. \\ &\left. + \frac{g}{4}\left[x^4 + 4x^3(x'-x_0) + 6x^2(x'-x_0)^2 + 4x(x'-x_0)^3 + (x'-x_0)^4\right]\right\}. \end{aligned} \tag{5.64}$$

Using formula (5.41) we obtain

$$V_{a^2}(x_0) = \frac{x_0^2}{2} + \frac{g}{4}x_0^4 + \frac{a^2}{2} + \frac{3}{2}gx_0^2a^2 + \frac{3g}{4}a^4. \tag{5.65}$$

From now on we shall always use natural units with $M = 1, \hbar = k_B = 1$, for convenience. Differentiating (5.65) with respect to $a^2/2$ gives, by (5.58),

$$\Omega^2(x_0) = \left(1 + 3gx_0^2 + 3ga^2\right). \tag{5.66}$$

We now solve this equation together with (5.56)

$$a^2(x_0) = \frac{1}{\beta\Omega^2(x_0)}\left(\frac{\beta\Omega(x_0)}{2}\coth\frac{\beta\Omega(x_0)}{2} - 1\right) \tag{5.67}$$

at each x_0, by iteration, starting out with $\Omega = 0$, inserting this into (5.67) to get $a^2 = \beta/12$, calculating from (5.66) an improved $\Omega^2(x_0)$, and so on. The iteration converges rapidly. Inserting the final $a^2(x_0)$, $\Omega^2(x_0)$ into (5.65) and (5.51), we obtain our approximation for the effective classical potential. By doing the integrals over x_0 we find the approximation Z_1 to the partition function Z. The associated free energies

$$F_1 = -\frac{1}{\beta}\ln Z_1 \tag{5.68}$$

are plotted as a function of β. For the detailed discussion of this application, see the next chapter.

Application to Double-Well Potential

A further example is the anharmonic oscillator with a negative harmonic term, the *double-well potential* [Feynman and Kleinert 1986, Janke and Kleinert 1986]

$$V(x) = -\frac{x^2}{2} + \frac{1}{4}gx^4. \tag{5.69}$$

The smeared potential $V_{a^2}(x_0)$ is the same form as in (5.65), except for a sign change in the first and third terms. In this case, the trial frequency

$$\Omega^2(x_0) \;=\; -1 + 3gx_0^2 + 3ga^2, \tag{5.70}$$

can become negative, although it remains always larger than $-4\pi^2/\beta^2$, i.e., it remains to the right of the first singularity in the sum (5.35). Thus the smearing width a^2 remains always positive. For $\Omega^2 \,\varepsilon\, \left(-4\pi^2/\beta^2, 0\right)$, the sum (5.35) gives

$$\begin{aligned} a^2(x_0) &= \frac{2}{\beta}\sum_{m=1}^{\infty}\frac{1}{\omega_m^2 + \Omega^2(x_0)} \\ &= \frac{1}{\beta\Omega^2(x_0)}\left(\frac{\beta|\Omega(x_0)|}{2}\cot\frac{\beta|\Omega(x_0)|}{2} - 1\right). \end{aligned} \tag{5.71}$$

This is, of course, the expression (5.67) analytically continued to imaginary $\Omega(x_0)$. The above procedure for finding the $a^2(x_0)$ and $\Omega^2(x_0)$ by iteration of (5.70) and (5.71) or (5.67) is not applicable near the central peak of the double well where it does not converge. But it is easy to find the solution by searching for the zero of the function of Ω^2

$$f\left(\Omega^2\right) \;\equiv\; a^2(x_0) - \frac{1}{3g}\left(1 + \Omega^2 - 3gx_0^2\right). \tag{5.72}$$

with $a^2(x_0)$ calculated as a function of Ω^2 from (5.71) or (5.67).

There are some other applications made use of this approximation, such as the particle distributions[Kleinert 1986, Janke and Kleinert 1986] and the Coulomb-Yukawa potential[Janke and Kleinert 1986].

New Improvement to Variational Approximation

Recently, Kleinert has improved the Feynman-Kleinert approximation to increase the power of the accuracy. The first improvement is given by introducing a separate trial frequency for each principle quantum number of a quantum system and apply it to the calculation of all energy levels of anharmonic oscillator[Kleinert 1992]. Another type[Kleinert 1993] of improvement is based on the expanding the action into powers of the fluctuation path around the average position and extending the action by bilocal external source. However, at this point we do not give in detail for those two improvement. Now we focus our attention to the other method of his improvement [Kleinert 1993] because it is greatly superior to any other ones. This method requires the evaluation of only a few correlation function and yields, for the anharmonic oscillator, extremely good approximation for all coupling constant g including the strong coupling limit. The process of this is as following

Firstly we expand the potential $V(x)$ by Taylor series around the mean point x_0 for each path.

$$
\begin{aligned}
V(x) &= V(x_0) + (x - x_0)\, V'(x_0) + \frac{1}{2!}(x - x_0)^2\, V''(x_0) \\
&\quad + \frac{1}{3!}(x - x_0)^3 V'''(x_0) + \ldots
\end{aligned}
\tag{5.73}
$$

Thus, the action S can be written as

$$
\begin{aligned}
S &= \int_0^{\beta\hbar} d\tau\, V(x_0) + \int_0^{\beta\hbar} d\tau \Big[\frac{1}{2!}(x - x_0)^2\, V''(x_0) + \ldots\Big] \\
&= \beta\hbar V(x_0) + S^{x_0} \\
&= S_0 + S^{x_0}.
\end{aligned}
\tag{5.74}
$$

Notice that the time integral of the second term of expansion vanish because of the definition of x_0 in (5.8). Now we can split the action S_0 into the local trial action $S_\Omega^{x_0}$ plus the interaction action $S_{\rm int}^{x_0}$ then we have

$$
S = S_0 + S_\Omega^{x_0} + S_{\rm int}^{x_0} \tag{5.75}
$$

where

$$S_{\Omega}^{x_0} = \int_0^{\beta\hbar} d\tau \left[\frac{M}{2}\dot{x}^2 + \frac{M}{2}\Omega^2(x_0)(x - x_0)^2\right] \tag{5.76}$$

with $\Omega(x_0)$ as the trial frequency and also parameter of the optimization.

The local partition function Z^{x_0} can be expressed as

$$\begin{aligned} Z^{x_0} &= \int \mathcal{D}x\bar{\delta}(x - x_0)e^{-S/\hbar} \\ &= e^{-S_0/\hbar}\int \mathcal{D}x\bar{\delta}(x - x_0)e^{-S_{\Omega}^{x_0}/\hbar}e^{-S_{\rm int}^{x_0}/\hbar} \\ &= e^{-S_0/\hbar}Z_{\Omega}^{x_0}\left\langle e^{-S_{\rm int}^{x_0}/\hbar}\right\rangle_{\Omega}^{x_0} \end{aligned} \tag{5.77}$$

with $Z_{\Omega}^{x_0}$ as the trial partition function, $\bar{\delta}(\bar{x} - x_0) = \sqrt{2\pi\beta\hbar / M}\,\delta(\bar{x} - x_0)$ as a modified δ -function which forces $\bar{x}$ to be equal to x_0, and $\langle\cdot\cdot\cdot\rangle_{\Omega}^{x_0}$ as the expectation calculated with the local trial partition function $Z_{\Omega}^{x_0}$. After expanding the exponential $\exp\{-S_{\rm int}^{x_0}/\hbar\}$ into a power series and using of the third cumulant expansion

$$\begin{aligned} \langle e^x\rangle &= exp\Big\{\langle x\rangle + \tfrac{1}{2}[\langle x^2\rangle - \langle x\rangle^2] \\ &\quad - \tfrac{1}{6}[\langle x^3\rangle - 3\langle x^2\rangle\langle x\rangle + 2\langle x\rangle^3]\Big\}, \end{aligned} \tag{5.78}$$

from (5.77) we obtain

$$Z^{x_0} \equiv e^{-\beta W_3^{x_0}}$$

$$\equiv \exp\left\{-\beta V(x_0) - \beta V_{\Omega}^{x_0} - \frac{1}{\hbar}\left\langle S_{\rm int}^{x_0}\right\rangle_{\Omega}^{x_0} + \frac{1}{2\hbar^2}\left\langle S_{\rm int}^{x_0\,2}\right\rangle_{\Omega,\,c}^{x_0} - \frac{1}{6\hbar^3}\left\langle S_{\rm int}^{x_0\,3}\right\rangle_{\Omega,\,c}^{x_0}\right\} \tag{5.79}$$

where the subscript c defines the connected correlation functions via the cumulant expansion

$$\left\langle S_{\rm int}^{x_0\,2} \right\rangle_{\Omega,\,c}^{x_0} \equiv \left\langle S_{\rm int}^{x_0\,2} \right\rangle_{\Omega}^{x_0} - \left\langle S_{\rm int}^{x_0} \right\rangle_{\Omega}^{x_0^2}$$

$$\left\langle S_{\rm int}^{x_0\,3} \right\rangle_{\Omega,\,c}^{x_0} \equiv \left\langle S_{\rm int}^{x_0\,3} \right\rangle_{\Omega}^{x_0} - 3\left\langle S_{\rm int}^{x_0\,2} \right\rangle_{\Omega}^{x_0} \left\langle S_{\rm int}^{x_0} \right\rangle_{\Omega}^{x_0} + 2\left\langle S_{\rm int}^{x_0} \right\rangle_{\Omega}^{x_0^3}, \qquad (5.80)$$

where $W_3^{x_0}$ defines the approximate effective classical potential corresponding to this method. We may carry the expansion further, but for this purpose we shall go only this far. The approximate local free energy of the system is obtained by extremizing $W_3^{x_0}$. defined by (5.79) with respect to the trial frequency Ω. The original Feynman-Kleinert approximation corresponds to stopping after the first expectation of $S_{\rm int}^{x_0}$.

To see the greatly improved accuracy brought about by the new terms consider first the partition function of the simple integral

$$Z = \int_{-\infty}^{\infty} \frac{dx_0}{\sqrt{2\pi/\beta\omega^2}} e^{-\beta(\omega^2 x_0^2/2 + g x_0^4/4)}. \qquad (5.81)$$

For convenience we may drop the locality label x_0, consider the interaction action

$$S_{\rm int}^{x_0} = S^{x_0} - S_{\Omega}^{x_0}$$

$$= \int_0^{\beta\hbar} d\tau \left[\frac{M}{2}\omega^2 x_0^2 - \frac{M}{2}\Omega^2 x_0^2 + \frac{1}{4} g x_0^4\right]$$

$$= \beta\hbar g\left(r x_0^2 + x_0^4\right)/4 \qquad (5.82)$$

with $r = 2M\left(\omega^2 - \Omega^2\right)/g$. The correlation function are simply

$$\langle S_{\rm int}\rangle_\Omega = g\left(3a^4 + r a^2\right)/4$$

$$\langle S_{\rm int}^2\rangle_{\Omega,\,c} \;=\; g^2\left(6a^8+3a^6r/2+a^4r^2/8\right)$$

$$\langle S_{\rm int}^3\rangle_{\Omega,\,c} \;=\; g^3\left(1188a^{12}+288a^{10}r+27a^8r^2+a^6r^3\right)/8 \qquad (5.83)$$

with

$$a^2 = 1/\beta M\Omega^2.$$

Let us finally illustrate the quality of the new approximation for the path integral of the anharmonic oscillator. For simplicity we consider only the worst possible case of a vanishing temperature. Then x_0 is equal to zero and can be dropped in all equations, the value of W_3 at x_0 giving an approximation E_3^0 for the ground state energy. The correlation function (5.83) of the interaction entering into W_3 of (5.80) become

$$\langle S_{\rm int}\rangle_\Omega = \hbar\beta g\left(3a^4+ra^2\right)/4$$

$$\langle S_{\rm int}^2\rangle_{\Omega,\,c} = \hbar\beta 2g^2\left(21a^8/8+3a^6r/4+a^4r^2/16\right)/\hbar\Omega$$

$$\langle S_{\rm int}^3\rangle_{\Omega,\,c} = \hbar\beta 6g^3\left(333a^{12}/16+105a^{10}r/16+3a^8r^2/4+a^6r^3/32\right)/\hbar^2\Omega^2. \qquad (5.84)$$

The r^n-terms are found from those with no r by replacing in their Ω by $\sqrt{\Omega^2+gr/2M}$ and expanding everything in power of r up to r^3.

For all detailed discussion of this chapter, see the next chapter.