
PERTURBATIVELY DEFINED PATH INTEGRAL IN PHASE SPACE

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Introducing a perturbative definition, phase space path integrals can be calculated without slicing. This leads to a short-time expansion of the quantum mechanical path amplitude or a high-temperature expansion of the unnormalized density matrix. We use the proposed formalism to calculate the effective classical Hamiltonian for the harmonic oscillator.

1 Introduction

Path integrals are usually evaluated by time-slicing [1], since the continuum definition is mathematically problematic. This becomes obvious for physical systems with nontrivial metric where reparametrization invariance has been a problem for many years [2]. It was solved recently by Kleinert and Chervyakov who defined path integrals perturbatively in *configuration space* [3] using dimensional regularization methods developed in the quantum theory of non-Abelian gauge fields [4]. They found rules for calculating integrals over products of distributions which establish a unique procedure for a perturbative evaluation of path integrals which fully respects parameterization invariance. The path integral of any system is expanded around the exactly known solution for the free particle in powers of the coupling constant of the potential.

In this article we want to present an extension of this definition to *phase space* and derive a short-time expansion of the Hamiltonian quantum mechanical time evolution amplitude. In Euclidean space, the density matrix is obtained as a high-temperature expansion. By simple resummation, this

series can be turned into an expansion in powers of the coupling constant of the potential described above. As will be shown in the sequel, the knowledge of an exactly known nontrivial path integral as that of a free particle is *not* required. Thus, the perturbative definition presented here is completely general. It reproduces the expansion around the free particle by a simple resummation.

The method is then applied to calculate the effective classical Hamiltonian of the harmonic oscillator $H_{\omega,\text{eff}}(p_0, x_0)$ by exactly summing up the perturbation series. The quantity is related to the quantum statistical partition function via the classically looking phase space integral

$$Z_\omega = \int \frac{dx_0 dp_0}{2\pi\hbar} \exp\{-\beta H_{\omega,\text{eff}}(p_0, x_0)\}, \quad (1)$$

where $\beta = 1/k_B T$ is the inverse thermal energy.

2 Perturbative Definition of the Path Integral for the Density Matrix

After slicing the interval $[0, \hbar\beta]$ into $N+1$ pieces of width $\varepsilon = \hbar\beta/(N+1)$, the unnormalized density matrix can be expressed in the continuum limit as [1]

$$\begin{aligned} \tilde{\rho}(x_b, x_a) &= \lim_{N \rightarrow \infty} \prod_{n=1}^N \left[\int_{-\infty}^{\infty} dx_n \right] \prod_{n=1}^{N+1} \left[\int_{-\infty}^{\infty} \frac{dp_n}{2\pi\hbar} e^{ip_n(x_n - x_{n-1})/\hbar} \right] \\ &\times \exp \left\{ -\varepsilon \sum_{n=1}^{N+1} H(p_n, x_n)/\hbar \right\}, \end{aligned} \quad (2)$$

where $x_a = x_0$ and $x_b = x_{N+1}$ are the fixed end points of the path. Upon expanding the last exponential in powers of ε/\hbar , we recognize that the zeroth-order contribution to the density matrix (2) is an *infinite product of δ -functions* due to the identity

$$\int_{-\infty}^{\infty} \frac{dp_n}{2\pi\hbar} e^{ip_n(x_n - x_{n-1})/\hbar} = \delta(x_n - x_{n-1}). \quad (3)$$

This infinite product simply reduces to

$$\lim_{N \rightarrow \infty} \int_{-\infty}^{\infty} dx_N \cdots dx_1 \delta(x_{N+1} - x_N) \cdots \delta(x_2 - x_1) \delta(x_1 - x_0) = \delta(x_b - x_a), \quad (4)$$

which is the unperturbed contribution to the unnormalized density matrix (2) obtained here without solving a nontrivial path integral. Thus, the phase space path integral for the unnormalized density matrix (2) can be perturbatively defined as

$$\begin{aligned} \tilde{\rho}(x_b, x_a) = & \delta(x_b - x_a) + \sum_{n=1}^{\infty} \frac{(-1)^n}{\hbar^n n!} \int_0^{\hbar\beta} d\tau_1 \cdots \int_0^{\hbar\beta} d\tau_n \\ & \times \langle H(p(\tau_1), x(\tau_1)) \cdots H(p(\tau_n), x(\tau_n)) \rangle_0 \end{aligned} \quad (5)$$

with expectation values

$$\langle \cdots \rangle_0 = \lim_{N \rightarrow \infty} \prod_{n=1}^N \left[\int_{-\infty}^{\infty} dx_n \right] \prod_{n=1}^{N+1} \left[\int_{-\infty}^{\infty} \frac{dp_n}{2\pi\hbar} \cdots e^{ip_n(x_n - x_{n-1})/\hbar} \right]. \quad (6)$$

These expectation values may be reexpressed by Feynman diagrams. This is possible for polynomial as well as nonpolynomial functions of momentum and position [5].

3 Restricted Partition Function and Two-Point Correlations

The trace over the unnormalized density matrix (5) of our unperturbed system with vanishing Hamiltonian $H(p, x) = 0$ leads to a diverging partition function. In addition, the classical partition function diverges with the phase space volume. The regularization of these divergences is possible by excluding, from the phase space path integral, the zero frequency fluctuations x_0 and p_0 of the Fourier decomposition of the periodic path $x(\tau)$ and momentum $p(\tau)$, respectively [1,6]. At the end, we shall calculate the quantum statistical partition function of any system from the classical phase space integral

$$Z = \int \frac{dx_0 dp_0}{2\pi\hbar} Z^{p_0 x_0}. \quad (7)$$

The restricted partition function in the integrand contains the Boltzmann factor of the effective classical Hamiltonian defined by the path integral:

$$\begin{aligned} Z^{p_0 x_0} \equiv & \exp \{ -\beta H_{\text{eff}}(p_0, x_0) \} = 2\pi\hbar \oint \mathcal{D}x \mathcal{D}p \delta(x_0 - \bar{x}) \delta(p_0 - \bar{p}) \\ & \times \exp \left\{ -\frac{1}{\hbar} \int_0^{\hbar\beta} d\tau \left[-i(p(\tau) - p_0) \frac{\partial}{\partial \tau} (x(\tau) - x_0) + H(p(\tau), x(\tau)) \right] \right\} \end{aligned} \quad (8)$$

with the measure

$$\oint \mathcal{D}x \mathcal{D}p = \lim_{N \rightarrow \infty} \prod_{n=1}^{N+1} \left[\int_{-\infty}^{\infty} \frac{dx_n dp_n}{2\pi\hbar} \right]. \quad (9)$$

The quantities \bar{x} and \bar{p} are the temporal mean values $\bar{x} = \int_0^{\hbar\beta} d\tau x(\tau)/\hbar\beta$ and $\bar{p} = \int_0^{\hbar\beta} d\tau p(\tau)/\hbar\beta$.

As illustrated above, the unperturbed system may have a vanishing Hamiltonian H . The calculation of the restricted partition function for this system to be denoted by $Z_0^{p_0 x_0}$, is *trivial* as for its density matrix in Eq. (4). A cancellation of δ -functions yields directly $Z_0^{p_0 x_0} = 1$.

Let us now concentrate on the correlation functions of position- and momentum-dependent quantities. For this purpose it is convenient to introduce the generating functional

$$\begin{aligned} Z_0^{p_0 x_0}[j, v] &= 2\pi\hbar \oint \mathcal{D}x \mathcal{D}p \delta(x_0 - \bar{x}) \delta(p_0 - \bar{p}) \\ &\times \exp \left\{ -\frac{1}{\hbar} \int_0^{\hbar\beta} d\tau \left[-i\tilde{p}(\tau) \frac{\partial}{\partial \tau} \tilde{x}(\tau) + j(\tau) \tilde{x}(\tau) + v(\tau) \tilde{p}(\tau) \right] \right\}, \end{aligned} \quad (10)$$

with abbreviations $\tilde{x}(\tau) = x(\tau) - x_0$ and $\tilde{p}(\tau) = p(\tau) - p_0$. The action in the exponent contains only the trivial Euclidean eikonal $S = -i \int d\tau \tilde{p} \partial \tilde{x} / \partial \tau$. The calculation yields

$$Z_0^{p_0 x_0}[j, v] = \exp \left\{ \frac{1}{\hbar^2} \int_0^{\hbar\beta} d\tau \int_0^{\hbar\beta} d\tau' j(\tau) G^{p_0 x_0}(\tau, \tau') v(\tau') \right\}, \quad (11)$$

where the periodic Green function is

$$\begin{aligned} G^{p_0 x_0}(\tau, \tau') &= -\frac{i}{2\beta} \{2(\tau - \tau') - \hbar\beta [\Theta(\tau - \tau') - \Theta(\tau' - \tau)]\} \\ &= \frac{2i}{\beta} \sum_{m=1}^{\infty} \frac{\sin \omega_m(\tau - \tau')}{\omega_m}. \end{aligned} \quad (12)$$

In the last line the Fourier decomposition is given with respect to Matsubara frequencies $\omega_m = 2\pi m/\hbar\beta$, omitting the zero mode. Observe the antisymmetry $G^{p_0 x_0}(\tau, \tau') = -G^{p_0 x_0}(\tau', \tau)$.

These Green functions possess an interesting scaling property: Substituting $\bar{\tau} \equiv \tau/\beta$, they become *independent* of β :

$$G^{p_0 x_0}(\bar{\tau}, \bar{\tau}') = -\frac{i}{2} \{2(\bar{\tau} - \bar{\tau}') - \hbar [\Theta(\bar{\tau} - \bar{\tau}') - \Theta(\bar{\tau}' - \bar{\tau})]\}. \quad (13)$$

Introducing expectation values as

$$\langle \dots \rangle_0^{p_0 x_0} = 2\pi\hbar \oint \mathcal{D}x \mathcal{D}p \delta(x_0 - \bar{x}) \delta(p_0 - \bar{p}) \cdots \exp \left\{ \frac{1}{\hbar} \int_0^{\hbar\beta} d\tau i\tilde{p}(\tau) \frac{\partial}{\partial \tau} \tilde{x}(\tau) \right\}, \quad (14)$$

the two-point functions are obtained from the functional (10) by performing appropriate functional derivatives with respect to $j(\tau)$ and $v(\tau)$, respectively:

$$\langle \tilde{x}(\tau) \tilde{x}(\tau') \rangle_0^{p_0 x_0} = 0, \quad (15)$$

$$\langle \tilde{x}(\tau) \tilde{p}(\tau') \rangle_0^{p_0 x_0} = G^{p_0 x_0}(\tau, \tau'), \quad (16)$$

$$\langle \tilde{p}(\tau) \tilde{p}(\tau') \rangle_0^{p_0 x_0} = 0. \quad (17)$$

The off-diagonal nature of the trivial action in (14) entails that only *mixed* position-momentum correlations do not vanish.

4 Perturbative Expansion for Effective Classical Hamiltonian

Expanding the restricted partition function (8) in powers of the Hamiltonian,

$$\begin{aligned} Z^{p_0 x_0} &= 1 + \sum_{n=1}^{\infty} \frac{(-1)^n}{\hbar^n n!} \int_0^{\hbar\beta} d\tau_1 \cdots \int_0^{\hbar\beta} d\tau_n \\ &\times \langle H(p(\tau_1), x(\tau_1)) \cdots H(p(\tau_n), x(\tau_n)) \rangle_0^{p_0 x_0}, \end{aligned} \quad (18)$$

rewriting this into a cumulant expansion, and utilizing the relation (8) between restricted partition function and effective classical Hamiltonian, we obtain

$$\begin{aligned} H_{\text{eff}}(p_0, x_0) &= \frac{1}{\beta} \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{\hbar^n n!} \int_0^{\hbar\beta} d\tau_1 \cdots \int_0^{\hbar\beta} d\tau_n \\ &\times \langle H(p(\tau_1), x(\tau_1)) \cdots H(p(\tau_n), x(\tau_n)) \rangle_{0,c}^{p_0 x_0}. \end{aligned} \quad (19)$$

Using Wick's rule, all correlation functions can be expressed in terms of products of two-point functions. Since only mixed two-point functions (12) can lead to nonvanishing contributions to the effective classical Hamiltonian, we

use the rescaled version (13) of the Green function. The scaling transformation gives a factor β from each of the n integral measures. Thus the expansion (19) is a *high-temperature* expansion of the effective classical Hamiltonian:

$$H_{\text{eff}}(p_0, x_0) = \sum_{n=1}^{\infty} \beta^{n-1} \frac{(-1)^{n+1}}{\hbar^n n!} \int_0^{\hbar} d\bar{\tau}_1 \cdots \int_0^{\hbar} d\bar{\tau}_n \times \langle H(p(\bar{\tau}_1), x(\bar{\tau}_1)) \cdots H(p(\bar{\tau}_n), x(\bar{\tau}_n)) \rangle_{0,c}^{p_0 x_0}. \quad (20)$$

For the following considerations it is useful to assume the Hamilton function to be of standard form:

$$H(p(\bar{\tau}), x(\bar{\tau})) = p^2(\bar{\tau})/2M + gV(x(\bar{\tau})). \quad (21)$$

We have introduced the coupling constant g of the potential. Defining the functionals

$$a[p] = \int_0^{\hbar} d\bar{\tau} p^2(\bar{\tau})/2M, \quad b[x] = \int_0^{\hbar} d\bar{\tau} V(x(\bar{\tau})), \quad (22)$$

the high-temperature expansion (20) is expressed as

$$H_{\text{eff}}(p_0, x_0) = \sum_{n=1}^{\infty} \beta^{n-1} \frac{(-1)^{n+1}}{n! \hbar^n} \sum_{k=0}^n g^k \binom{n}{k} \langle a^{n-k}[p] b^k[x] \rangle_{0,c}^{p_0 x_0}. \quad (23)$$

In the sequel we point out how this high-temperature expansion is connected with an expansion in powers of the coupling constant g of the potential.

5 High-Temperature Versus Weak-Coupling Expansion

Having shown that the perturbative expansion around a vanishing Hamiltonian leads to a perturbative series in powers of the inverse temperature in a natural manner, we now elaborate on its relation to more customary perturbative expansions in powers of the coupling constant g of the potential. Changing the order of summation in Eq. (23), we obtain

$$H_{\text{eff}}(p_0, x_0) = \sum_{k=0}^{\infty} g^k \sum_{n=0}^{\infty} \beta^{n+k-1} \binom{n+k}{k} \frac{(-1)^{n+k+1}}{(n+k)! \hbar^{n+k}} \langle a^n[p] b^k[x] \rangle_{0,c}^{p_0 x_0} + \frac{1}{\beta}, \quad (24)$$

which is rewritten after explicitly evaluating the contributions for $n = 0$ and $k = 0$:

$$\begin{aligned}
 H_{\text{eff}}(p_0, x_0) &= \frac{p_0^2}{2M} + gV(x_0) + \frac{1}{\beta} \sum_{k=1}^{\infty} g^k \sum_{n=1}^{\infty} \frac{(-1)^{n+k+1}}{n!k!\hbar^{n+k}(2M)^n} \\
 &\times \int_0^{\hbar\beta} d\tau_1 \cdots \int_0^{\hbar\beta} d\tau_k \int_0^{\hbar\beta} d\tau_{k+1} \cdots \int_0^{\hbar\beta} d\tau_{k+n} \\
 &\times \langle V(x(\tau_1)) \cdots V(x(\tau_k)) p^2(\tau_{k+1}) \cdots p^2(\tau_{k+n}) \rangle_{0,c}^{p_0 x_0}. \quad (25)
 \end{aligned}$$

In this expression, we have inverted the scaling transformation in (13) and used the expectation values

$$\int_0^{\hbar\beta} d\tau \langle p^2(\tau) \rangle_{0,c}^{p_0 x_0} = \hbar\beta p_0^2, \quad \int_0^{\hbar\beta} d\tau \langle V(x(\tau)) \rangle_{0,c}^{p_0 x_0} = \hbar\beta V(x_0). \quad (26)$$

All higher-order expectations of functions which only depend on x or p are zero, due to the vanishing of expectations of functions of \tilde{x} or \tilde{p} in a Wick expansion into products of two-point functions (15) and (17). All other possible contributions are disconnected.

We now observe that the expansion (25) is equal to a perturbation expansion around a free-particle theory

$$\begin{aligned}
 H_{\text{eff}}(p_0, x_0) &= \frac{p_0^2}{2M} + gV(x_0) + \frac{1}{\beta} \sum_{k=1}^{\infty} g^k \frac{(-1)^{k+1}}{k!\hbar^k} \int_0^{\hbar\beta} d\tau_1 \cdots \int_0^{\hbar\beta} d\tau_k \\
 &\times \langle V(x(\tau_1)) \cdots V(x(\tau_k)) \rangle_{\text{free},c}^{x_0}, \quad (27)
 \end{aligned}$$

in which cumulants are formed from expectation values

$$\begin{aligned}
 \langle \cdots \rangle_{\text{free}}^{x_0} &= 2\pi\hbar \oint \mathcal{D}x \mathcal{D}p \delta(x_0 - \bar{x}) \delta(p_0 - \bar{p}) \cdots \\
 &\times \exp \left\{ -\frac{1}{\hbar} \int_0^{\hbar\beta} d\tau \left[-i(p(\tau) - p_0) \frac{\partial}{\partial \tau} (x(\tau) - x_0) + \frac{1}{2M} (p(\tau) - p_0)^2 \right] \right\}. \quad (28)
 \end{aligned}$$

creates a new subgraph which contains a propagator (30) or (31), respectively. These propagators are, however, independent of τ , such that the τ -integrals related to the vertices in these subgraphs are trivial. Thus, there does not really exist a connection between these vertices, and the propagators (30) and (31) can be expressed by the currents (34) and (35):

$$\bar{\tau}_1 \text{ --- } \bar{\tau}_2 = \bar{\tau}_1 \text{ --- } \star \text{ --- } \bar{\tau}_2, \quad (40)$$

$$\bar{\tau}_1 \text{ --- } \bar{\tau}_2 = \bar{\tau}_1 \text{ --- } \star \text{ --- } \bar{\tau}_2. \quad (41)$$

As a consequence, connected diagrams for $n > 1$ containing propagators of type (30) or (31) *must* break up into disconnected parts. Analytically, this is seen by considering for example

$$\langle x(\bar{\tau}_1)x(\bar{\tau}_2) \rangle_0^{p_0x_0} = \langle \tilde{x}(\bar{\tau}_1)\tilde{x}(\bar{\tau}_2) \rangle_0^{p_0x_0} + \langle x(\bar{\tau}_1) \rangle_0^{p_0x_0} \langle x(\bar{\tau}_2) \rangle_0^{p_0x_0}. \quad (42)$$

The first term on the right-hand side vanishes due to Eq. (15), while the second simply yields x_0^2 , which proves Eq. (33). This means that only Feynman diagrams which consist of a mixture of subgraphs (37) and (38) contribute to the effective classical Hamiltonian. To illustrate this, we discuss the first and second order of expansion (20) in more detail.

The Feynman diagrams of the first-order contribution to the effective classical Hamiltonian are simply constructed from the subgraphs

$$\begin{aligned} H_{\omega,\text{eff}}^{(1)}(p_0, x_0) &\propto \text{---} \text{---} + \text{---} \text{---} \\ &= \frac{1}{2M\hbar} \text{---} \text{---} + \frac{1}{2\hbar} M\omega^2 \text{---} \text{---} = \frac{1}{2M\hbar} \text{---} \text{---} \star \text{---} \text{---} + \frac{1}{2\hbar} M\omega^2 \text{---} \text{---} \star \text{---} \text{---} \\ &= \frac{p_0^2}{2M} + \frac{1}{2} M\omega^2 x_0^2, \end{aligned} \quad (43)$$

where we have used the identities (40) and (41) in the second expression of the second line. Note that the first-order term (43) obviously reproduces the classical Hamiltonian. This is the consequence of the high-temperature expansion (23), since only the first-order contribution is nonzero in the limit $\beta = 1/k_B T \rightarrow 0$. The second-order contribution reads

$$\begin{aligned} H_{\omega,\text{eff}}^{(2)}(p_0, x_0) &\propto (\text{---} \text{---} + \text{---} \text{---}) (\text{---} \text{---} + \text{---} \text{---}) \\ &= -\frac{\omega^2}{8\hbar^2\beta} \left(8 \text{---} \text{---} \star \text{---} \text{---} + 4 \text{---} \text{---} \right). \end{aligned} \quad (44)$$

The chain diagram is zero, while the loop diagram has the value $-\hbar^4\zeta(2)/2\pi^2$,

where $k = n/2$. The high-temperature expansion for the effective classical Hamiltonian of the harmonic oscillator can then be written as

$$H_{\omega,\text{eff}}(p_0, x_0) = \frac{p_0^2}{2M} + \frac{1}{2}M\omega^2 x_0^2 + \sum_{k=1}^{\infty} \beta^{2k-1} \frac{(-1)^{k+1}}{k} \left(\frac{\hbar\omega}{2\pi}\right)^{2k} \zeta(2k). \quad (49)$$

Substituting the ζ -function by its definition (45) and exchanging the summations, the last term in Eq. (49) can be expressed as a logarithm

$$\sum_{k=1}^{\infty} \beta^{2k-1} \frac{(-1)^{k+1}}{k} \left(\frac{\hbar\omega}{2\pi}\right)^{2k} \zeta(2k) = \frac{1}{\beta} \ln \left(\prod_{n=1}^{\infty} \left[1 + \frac{\hbar^2 \beta^2 \omega^2}{4\pi^2 n^2} \right] \right). \quad (50)$$

Applying the relation

$$\frac{1}{z} \sinh z = \prod_{n=1}^{\infty} \left(1 + \frac{z^2}{n^2 \pi^2} \right), \quad (51)$$

we find the more familiar form of the effective classical Hamiltonian for a harmonic oscillator

$$H_{\omega,\text{eff}}(p_0, x_0) = \frac{p_0^2}{2M} + \frac{1}{2}M\omega^2 x_0^2 - \frac{1}{\beta} \ln \frac{\hbar\omega\beta}{2 \sinh(\hbar\omega\beta/2)}. \quad (52)$$

When performing the x_0 - and p_0 -integrations in Eq. (1), we obtain the well-known form of the partition function of the harmonic oscillator $Z_{\omega} = 1/2 \sinh(\hbar\omega\beta/2)$.

7 Summary

We have used a perturbative definition of the path integral in phase space representation which produces an effective classical Hamiltonian for the harmonic oscillator. Our procedure represents an alternative way to evaluate path integrals: The unperturbed system is trivial and the calculation of appropriate Feynman diagrams is simple. As a further advantage, the perturbative expansion for the effective classical Hamiltonian is identical to the high-temperature expansion used frequently in statistical mechanics.

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