Lecture 3: PATH INTEGRALS IN QUANTUM MECHANICS

The path integral formalism, which we explain now in the context of quantum mechanics, leads to a representation of physical quantities as averages with an appropriate weight (real or complex) over a set of paths or trajectories. Thus, it gives a rather concrete meaning to the concept of quantum fluctuations.

In fact, to a large extent, one could define quantum mechanics directly in terms of path integrals, quite interesting a viewpoint, but which would require the introduction of a mathematical formalism more complicated than differential equations for the study even of simple quantum systems.

Note, however, that when the number of degrees of freedom is large, as in statistical physics or in quantum field theory, the advantage of the functional integral formalism becomes overwhelming.

Here instead, for pedagogical reasons, we assume some minimal background in quantum mechanics, as the notion of Hilbert space (the notation of bras and kets will be used for vectors), on which act hermitian or unitary operators corresponding to the physical observables, like position, momentum, the time evolution operator or the density matrix.

Moreover, the evolution of wave functions is governed by the Schrödinger equation.

We first describe a general strategy that leads to a representation of the matrix elements (in the position basis) of some evolution operators by path integrals. The existence of such a representation rely on two basic properties:

(i) A Markovian evolution, that is, without memory, a characteristic property of isolated systems or without influence on their environment.

(ii) The locality of the evolution for short time intervals, a property that we explain later. The locality of quantum evolution is in correspondence with the locality of classical evolution.

These two properties are satisfied both by the unitary evolution operator $e^{-itH/\hbar}$ (this form assumes that H is a time-independent Hamiltonian) that describes quantum evolution and the statistical operator $e^{-\beta H}$, which is proportional to the density matrix at thermal equilibrium.

They are also shared by some stochastic processes of diffusion type that are not related to quantum physics, like Brownian motion, which historically has led to the introduction of path integrals (Wiener's integral).

We then construct a path integral representation of the matrix elements of the statistical operator in the simple example of Hamiltonians of the form $H = \hat{p}^2/2m + V(\hat{q})$, where $\hat{q}$, $\hat{p}$ are the position and momentum operators, respectively.

3.1 Position, momentum operators and matrix elements

The notion of locality makes reference to positions. In quantum mechanics, to each physical observable, like position, is associated a hermitian operator. We introduce the basis in Hilbert space in which the position operator $\hat{q}$ is diagonal. The eigenvalues q of $\hat{q}$ are real and, in the standard bra and ket notation, the corresponding eigenvectors (in some extended sense) $|q\rangle$ are orthogonal:

$$\hat{q}\,|q\rangle = q\,|q\rangle\,, \quad \langle q'|q\rangle = \delta(q-q'). \tag{3.1}$$

(δ is Dirac's function). Moreover, the basis is complete, which implies

$$\int \mathrm{d}q\,|q\rangle\,\langle q| = \mathbf{1}\,. \tag{3.2}$$

In terms of matrix elements in this basis, using the decomposition (3.2) of the identity, one can write the product of two operators $\mathcal{O}_1$ and $\mathcal{O}_2$ as

$$\langle q''|\,\mathcal{O}_2\mathcal{O}_1\,|q'\rangle = \int \mathrm{d}q\,\langle q''|\,\mathcal{O}_2\,|q\rangle\,\langle q|\,\mathcal{O}_1\,|q'\rangle\,.$$

3.1.1 Momentum operator and Fourier transformation

We now assume that the position operator $\hat{\mathbf{q}}$ is a d-component vector ($\mathbf{q} \in \mathbb{R}^d$) and denote by $\hat{\mathbf{p}}$ the corresponding momentum operator. Their components have the canonical commutation relations

$$[\hat{q}_\alpha, \hat{p}_\beta] = i\hbar\delta_{\alpha\beta}\mathbf{1}\,.$$

($\mathbf{1}$ is the identity operator).

Fourier transformation: convention. Denoting by $|\widetilde{\mathbf{p}}\rangle$ the vectors of the basis in which the momentum operator $\hat{\mathbf{p}}$ is diagonal, we define the Fourier transformation by

$$\int \mathrm{d}^d q\ \mathrm{e}^{i\mathbf{q}\cdot\mathbf{p}/\hbar}\,|\mathbf{q}\rangle = |\widetilde{\mathbf{p}}\rangle. \tag{3.3}$$

The matrix elements of the identity operator in this basis are then

$$\langle\widetilde{\mathbf{p}}''|\,\mathbf{1}\,|\widetilde{\mathbf{p}}'\rangle = \langle\widetilde{\mathbf{p}}''\ |\widetilde{\mathbf{p}}'\rangle = (2\pi\hbar)^d\delta^{(d)}(\mathbf{p}''-\mathbf{p}').$$

Therefore, in a product of operators in momentum representation, the integration measure is $\mathrm{d}^d p/(2\pi\hbar)^d$:

$$\langle\widetilde{\mathbf{p}}''|\, U_2 U_1\, |\widetilde{\mathbf{p}}'\rangle = \int \frac{\mathrm{d}^d p}{(2\pi\hbar)^d}\, \langle\widetilde{\mathbf{p}}''|\, U_2\, |\widetilde{\mathbf{p}}\rangle\, \langle\widetilde{\mathbf{p}}|\, U_1\, |\widetilde{\mathbf{p}}'\rangle\, .$$

Moreover, this normalization implies for the wave functions $\psi(\mathbf{q}) \equiv \langle\mathbf{q}|\psi\rangle$:

$$\langle\widetilde{\mathbf{p}}|\,\psi\rangle \equiv \tilde{\psi}(\mathbf{p}) = \int \mathrm{d}^d q\, \mathrm{e}^{-i\mathbf{q}\cdot\mathbf{p}/\hbar}\, \psi(\mathbf{q}) \;\Rightarrow\; \psi(\mathbf{q}) = \frac{1}{(2\pi\hbar)^d} \int \mathrm{d}^d p\, \mathrm{e}^{i\mathbf{q}\cdot\mathbf{p}/\hbar}\, \tilde{\psi}(\mathbf{p}).$$

3.2 Markov process

We consider a bounded operator in a Hilbert space, $U(t, t')$, $t \geq t'$, which describes the evolution from time t' to time t and which satisfies a Markov property in time:

$$U(t, t'')U(t'', t') = U(t, t'), \text{ for } t \geq t'' \geq t' \text{ and } U(t', t') = \mathbf{1}\,. \tag{3.4}$$

This property, which is also characteristic of some stochastic processes, means that the evolution associated with the operator U has no memory. The evolution from time t'' to time t depends only on the state of the system at time t'', and not on the preceding evolution.

The Markov property (3.4) allows writing $U(t'', t')$ as a product, time-ordered as in equation (3.4), of operators corresponding to time intervals ε that we choose equal and which can be made arbitrarily small:

$$U(t'', t') = \prod_{m=1}^{n} U[t' + m\varepsilon, t' + (m-1)\varepsilon], \qquad \varepsilon = (t'' - t')/n\,. \tag{3.5}$$

When the evolution operator then takes the special form $U(t,t') \equiv U(t-t')$, the evolution is time-translation invariant and the Markov property (3.4) becomes a semi-group property: $U(t)U(t') = U(t+t')$ with $t \geq 0\,,\ t' \geq 0\,.$

3.2.1 Differentiable evolution operators

We assume now that $U(t,t')$ is differentiable with a continuous derivative. We set

$$\left.\frac{\partial U(t,t')}{\partial t}\right|_{t=t'} = -K(t)\,.$$

Differentiating equation (3.4) with respect to t and taking the $t'' = t$ limit, one finds

$$\frac{\partial U}{\partial t}(t,t') = -K(t)U(t,t')\,. \tag{3.6}$$

When the operator K is time-independent, it is the generator of time translations, $U(t+\varepsilon,t) = \mathrm{e}^{-\varepsilon K}$ and one recognizes in equation (3.5) Trotter's formula.

The operator K. In these lectures, we meet two types of operators:

If the operator U describes quantum evolution in time, it is unitary and the operator $K = iH/\hbar$ where H is the hermitian quantum Hamiltonian.

If the operator K itself is hermitian and time-independent, $K = H$ and the operator $U(\beta, 0)$ is the statistical quantum operator, proportional to the density matrix $\rho(\beta)$ at thermal equilibrium at a temperature $T = 1/\beta$ (the equilibrium can be induced by a weak coupling to a thermal bath):

$$\rho(\beta) = U(\beta, 0)/\mathcal{Z}(\beta), \quad \mathcal{Z}(\beta) = \operatorname{tr} U(\beta, 0)$$

and $\mathcal{Z}$ is the partition function.

Nevertheless, we will still call the evolution variable time (or Euclidean time), even though, from the viewpoint of quantum evolution, it is an imaginary time. Indeed, if one sets $\beta = it/\hbar$, one recovers the usual evolution operator of quantum mechanics. The same analytic continuation allows transposing the algebraic part of the calculations that follow to quantum evolution.

3.2.2 Matrix elements

Introducing matrix elements in the position basis, we can rewrite identity (3.4) for times $t_3 \geq t_2 \geq t_1$ as

$$\langle q_3 | U(t_3, t_1) | q_1 \rangle = \int \mathrm{d}q_2 \, \langle q_3 | U(t_3, t_2) | q_2 \rangle \langle q_2 | U(t_2, t_1) | q_1 \rangle ,$$

where we have used the decomposition (3.2) of the identity.

Generalizing this identity, we rewrite equation (3.5) as

$$\langle q'' | U(t'', t') | q' \rangle = \int \prod_{k=1}^{n-1} \mathrm{d}q_k \prod_{k=1}^{n} \langle q_k | U(t_k, t_{k-1}) | q_{k-1} \rangle \tag{3.7}$$

with the conventions

$$t_k = t' + k\varepsilon \, , \; q_0 = q' , \; q_n = q'' .$$

In this expression, we can take the limit $n \to \infty$, or $\varepsilon \to 0$, reducing the evaluation of expression (3.7) to the asymptotic evaluation (but with enough precision) of matrix elements $\langle q | U(t+\varepsilon, t) | q' \rangle$ for infinitesimal time intervals.

3.3 Locality of short-time evolution

Local short time evolution means that the support of the matrix elements $\langle q''|U(t'',t')|q'\rangle$ vanish for $|q''-q'|>0$ when $t''-t'$ goes to zero. An explicit and very relevant example is provided by the random walk where the role of $\langle q''|U(t'',t')|q'\rangle$ is played by the transition probability $\rho(q''-q')$ and, in macroscopic variables, for $t''-t'=\varepsilon \ll 1$,

$$\rho(q) \propto \mathrm{e}^{-q^2/2\varepsilon} .$$

Assuming that the operator U is differentiable, we have introduced its derivative $-K(t)$. If U is local, the matrix elements of the operator $\langle q''|K|q'\rangle$ have a support limited to $q'=q''$. This property is satisfied by differential operators, which can be represented by a polynomial in the momentum operator $\hat{p}$, $K(t)\equiv K(\hat{p},\hat{q};t)$. In what follows we mainly consider operators proportional to quantum Hamiltonians of the form $\hat{p}^2/2m+V(\hat{q})$, which clearly satisfy the locality condition.

3.3.1 Free evolution or Brownian motion

As an illustration, we first consider the example of the statistical operator corresponding to a free particle of mass m in d dimensions, which is mathematically equivalent to the example of Brownian motion already discussed.

The quantum Hamiltonian of the free motion can be written as

$$H_0 = \hat{\mathbf{p}}^2/2m\,.$$

The matrix elements of the operator $U(\beta,0) = \mathrm{e}^{-\beta H_0}$ are simple in the basis in which $\hat{\mathbf{p}}$ is diagonal since

$$\langle\widetilde{\mathbf{p}}''|\,U(\beta,0)\,|\widetilde{\mathbf{p}}'\rangle = \delta^{(d)}(\mathbf{p}''-\mathbf{p}')\,\mathrm{e}^{-\beta\mathbf{p}'^2}\,.$$

They are related with the position basis by Fourier transformation.

Inverting the Fourier transformation, one concludes

$$
\begin{aligned}
\langle \mathbf{q}'' \left| U(\beta,0) \right| \mathbf{q}' \rangle &= \int \frac{\mathrm{d}^d p}{(2\pi\hbar)^d} \exp\left(i \frac{(\mathbf{q}''-\mathbf{q}')\cdot\mathbf{p}}{\hbar} - \beta \frac{\mathbf{p}^2}{2m} \right) \\
&= \left(\frac{m}{2\pi\beta}\right)^{d/2} \exp\left(-\frac{m}{2\beta} \frac{(\mathbf{q}''-\mathbf{q}')^2}{\hbar^2} \right) .
\end{aligned}
\tag{3.8}
$$

The expression clearly exhibits a locality property: when $\beta \to 0$, the region in which $\langle \mathbf{q}''|U(\beta,0)|\mathbf{q}'\rangle$ remains finite decreases as $|\mathbf{q}''-\mathbf{q}'| = O(\sqrt{\beta})$.

3.3.2 The statistical operator for short time intervals

From now on, the operator K, which appears in equation (3.6), is identified with a quantum Hamiltonian of the form

$$
K \equiv H = \hat{\mathbf{p}}^2/2m + V(\hat{\mathbf{q}}) , \tag{3.9}
$$

(where $\mathbf{p}, \mathbf{q}$ are d-component vectors) where the potential V is differentiable and, temporarily, assumed to be time-independent.

Then, time-translation invariance implies $U(t'',t') = U(t''-t',0)$.

When the potential is differentiable, for short time intervals, one can use the Baker-Campbell-Hausdorff formula at leading order,

$$U(\varepsilon,0) = \mathrm{e}^{-\varepsilon H} = \mathrm{e}^{-\varepsilon\hat{p}^2/2m}\,\mathrm{e}^{-\varepsilon V(\hat{q})+O(\varepsilon^2)},$$

where the term of order ε^2 is proportional to the commutator $[\hat{p}^2, V(\hat{q})]$. Taking the matrix elements of both sides, one finds

$$\langle \mathbf{q}''|\,U(\varepsilon,0)\,|\mathbf{q}'\rangle = \left(\frac{m}{2\pi\varepsilon}\right)^{d/2} \exp\left[-\frac{m\,(\mathbf{q}''-\mathbf{q}')^2}{2\varepsilon\hbar^2} - \varepsilon V(\mathbf{q}')\right].$$

Basic observation. In the exponent, the most singular term for $\varepsilon \to 0$ is $(\mathbf{q}-\mathbf{q}')^2/2\varepsilon$ (which is independent of the potential). This implies that the support of the matrix element $\langle \mathbf{q}|U(\beta,0)|\mathbf{q}'\rangle$ corresponds to values $|\mathbf{q}'-\mathbf{q}| = O(\sqrt{\varepsilon})$, as in the Brownian motion.

Then, for $|\mathbf{q}' - \mathbf{q}| = O(\sqrt{\varepsilon})$,

$$\begin{aligned}\varepsilon V(\mathbf{q}') = \varepsilon V(\mathbf{q}) + O(\varepsilon^{3/2}) &= \tfrac{1}{2}\varepsilon\big(V(\mathbf{q}) + V(\mathbf{q}')\big) + O(\varepsilon^{3/2}) \\ &= \int_0^{\varepsilon} \mathrm{d}t\, V\big((\mathbf{q}' + (\mathbf{q} - \mathbf{q}')t/\varepsilon\big) + O(\varepsilon^{3/2}).\end{aligned}$$

Introducing the trajectory

$$\mathbf{q}(t) = (\mathbf{q}' + (\mathbf{q} - \mathbf{q}')t/\varepsilon$$

and the quantity $(\dot{\mathbf{q}}(t) \equiv \mathrm{d}\mathbf{q}/dt)$

$$\mathcal{S}(\varepsilon, 0) = \int_0^{\varepsilon} \mathrm{d}t\, \left[\frac{m}{2\hbar^2}\dot{\mathbf{q}}^2(t) + V\big(\mathbf{q}(t)\big)\right],$$

one can rewrite the matrix elements of the statistical operator

$$\langle \mathbf{q}|\, U(\varepsilon, 0)\, |\mathbf{q}'\rangle = \left(\frac{m}{2\pi\varepsilon}\right)^{d/2} \mathrm{e}^{-\mathcal{S}(\varepsilon,0) + O(\varepsilon^{3/2})}\,.$$

3.3.3 Path integral representation of the statistical operator

We now combine equation (3.7) in the form,

$$\langle \mathbf{q}'' \,|U(\beta,0)|\, \mathbf{q}' \rangle = \int \prod_{k=1}^{n-1} \mathrm{d}^d q_k \prod_{k=1}^{n} \langle \mathbf{q}_k \,|U(t_k,t_{k-1})|\, \mathbf{q}_{k-1} \rangle \,,$$

in the limit $n \to \infty$, $\varepsilon \to 0$ at $n\varepsilon = \beta$ fixed, where $t_k = k\varepsilon$, with the short time evaluation of the matrix elements of the statistical operator.

In terms of the piecewise linear, continuous trajectory,

$$\mathbf{q}(t) = \mathbf{q}_k + (\mathbf{q}_{k+1} - \mathbf{q}_k)(t - t_k)/\varepsilon \quad \text{for} \quad t_k \le t \le t_{k+1} \,,$$

we obtain

$$\langle \mathbf{q}'' \,|U(\beta,0)|\, \mathbf{q}' \rangle = \lim_{n\to\infty} \left(\frac{m}{2\pi\varepsilon}\right)^{dn/2} \int \prod_{k=1}^{n-1} \mathrm{d}^d q_k \; \mathrm{e}^{-\mathcal{S}(\mathbf{q},\varepsilon)}, \tag{3.10}$$

$$\text{with} \quad \mathcal{S}(\mathbf{q},\varepsilon) = \sum_{k=1}^{n} \mathcal{S}(t_k,t_{k-1}) + O(n\varepsilon^{3/2} = \beta\sqrt{\varepsilon}).$$

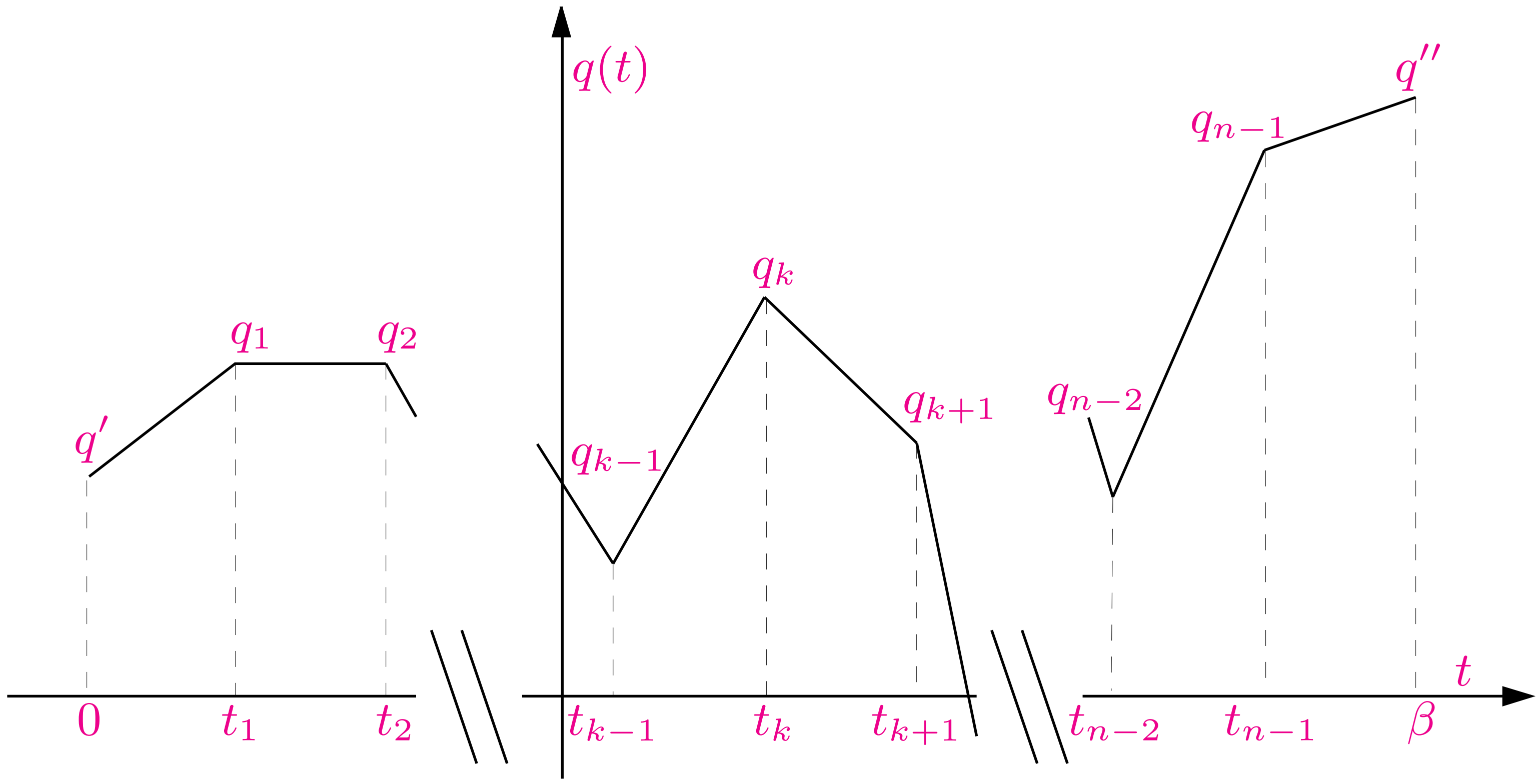

Fig. 3.1 – A path contributing to the integral (3.10): $\mathbf{q}_k \equiv \mathbf{q}(t_k)$.

The integration over the variables $\mathbf{q}_k$ is thus equivalent to an integration over the points of a piecewise linear path of the kind displayed in Fig. 3.1.

Summing over k, one obtains

$$\begin{aligned}\mathcal{S}(\mathbf{q},\varepsilon) &= \sum_{k=0}^{n-1}\int_{t_k}^{t_{k+1}} \mathrm{d}t\left[\frac{m}{2\hbar^2}\dot{\mathbf{q}}^2(t)+V\big(\mathbf{q}(t)\big)\right]+O(\beta\sqrt{\varepsilon})\\ &= \int_0^\beta \mathrm{d}t\left[\frac{m}{2\hbar^2}\dot{\mathbf{q}}^2(t)+V\big(\mathbf{q}(t)\big)\right]+O(\beta\sqrt{\varepsilon}).\end{aligned}$$

In the limit $n\to\infty$, $\varepsilon\to 0$ with $n\varepsilon=\beta$ fixed, $\mathcal{S}(\mathbf{q},\varepsilon)$ converges toward the action

$$\mathcal{S}(\mathbf{q}) \equiv \int_0^\beta \mathrm{d}t\left[\frac{m}{2\hbar^2}\dot{\mathbf{q}}^2(t)+V\big(\mathbf{q}(t)\big)\right]. \tag{3.11}$$

For $\hbar=1$, we recognize the integral of the Euclidean Lagrangian associated with the Hamiltonian. The Euclidean Lagrangian differs from the usual action of classical mechanics by the relative sign between the kinetic and potential terms.

From a formal viewpoint, the Euclidean action corresponds to a motion in imaginary time and this explains the sign difference.

We then take the formal limit of expression (3.10):

$$\langle \mathbf{q}'' \,| U(\beta, 0) |\, \mathbf{q}' \rangle = \int_{\mathbf{q}(0)=\mathbf{q}'}^{\mathbf{q}(\beta)=\mathbf{q}''} [\mathrm{d}\mathbf{q}(t)]\, \mathrm{e}^{-\mathcal{S}(\mathbf{q})}, \tag{3.12}$$

and call it path integral because the right hand side involves a sum over all paths satisfying the prescribed boundary conditions, with the weight $\mathrm{e}^{-\mathcal{S}(\mathbf{q})}$.

Remarks.

(*i*) We use the symbol $[\mathrm{d}\mathbf{q}(t)]$, with brackets, throughout these lectures, to distinguish path integrals from ordinary integrals.

(*ii*) We have assumed the potential time-independent but a little more labour one can show that the path integral representation is also valid for time-dependent potentials, a situation mainly relevant for real-time.

(iii) In the symbol $[\mathrm{d}\mathbf{q}(t)]$ is hidden a normalization

$$\mathcal{N} = \left(\frac{m}{2\pi\hbar\varepsilon}\right)^{dn/2}$$

that diverges for $n \to \infty$ but does not depend on the potential. Therefore, in explicit calculations, path integrals are generally normalized by dividing them by reference path integrals whose value is already known (the free motion $V \equiv 0$, for example).

(iv) In contrast to a more abstract construction of quantum mechanics, the path integral representation relies on a specific basis, the basis in which the position operator is diagonal.

Generalization. The generalization of the preceding construction to a system with several particles corresponding to a Hamiltonian

$$H=\sum_a \frac{\hat{\mathbf{p}}_a^2}{2m_a}+V(\hat{\mathbf{q}}),$$

is immediate and leads to a path integral

$$\langle \mathbf{q}''\,|U(t'',t')|\,\mathbf{q}'\rangle=\int_{\mathbf{q}(t')=\mathbf{q}'}^{\mathbf{q}(t'')=\mathbf{q}''}[\mathrm{d}\mathbf{q}(t)]\,\mathrm{e}^{-\mathcal{S}(\mathbf{q})},$$

which involves the corresponding action

$$\mathcal{S}(\mathbf{q})=\int \mathrm{d}t\left[\sum_a \frac{m_a}{2\hbar^2}\dot{\mathbf{q}}_a^2(t)+V\big(\mathbf{q}(t)\big)\right].$$

Euclidean or imaginary-time action. If the action we change variables, setting $t \mapsto \tau = \hbar t$, the path integral becomes

$$\langle \mathbf{q}'' \,|U(\tau'', \tau')|\, \mathbf{q}' \rangle = \int_{\mathbf{q}(\tau')=\mathbf{q}'}^{\mathbf{q}(\tau'')=\mathbf{q}''} [\mathrm{d}\mathbf{q}(\tau)]\, \mathrm{e}^{-\mathcal{S}_{\mathrm{E}}(\mathbf{q})/\hbar},$$

where $\mathcal{S}_{\mathrm{E}}(\mathbf{q})$ is now the Euclidean action,

$$\mathcal{S}_{\mathrm{E}}(\mathbf{q}) = \int_{\tau'}^{\tau''} \mathrm{d}\tau \,\left[\tfrac{1}{2} m \dot{\mathbf{q}}^2 + V\big(\mathbf{q}(\tau)\big)\right],$$

integral of the Euclidean Lagrangian.

3.3.4 Real-time or classical action

Finally, if instead we change variables, setting $t \mapsto \tau = -i\hbar t$, we obtain the matrix elements of the evolution operator,

$$\langle \mathbf{q}'' \left| U(t'', t') \right| \mathbf{q}' \rangle = \int_{\mathbf{q}(t')=\mathbf{q}'}^{\mathbf{q}(t'')=\mathbf{q}''} [\mathrm{d}\mathbf{q}(t)]\, \mathrm{e}^{i\mathcal{A}(\mathbf{q})/\hbar}, \tag{3.13}$$

where $\mathcal{A}$ is the usual classical action, integral of the classical Lagrangian:

$$\mathcal{A}(\mathbf{q}) = \int_{t'}^{t''} \mathrm{d}t \, \left[\tfrac{1}{2} m \dot{\mathbf{q}}^2 - V\big(\mathbf{q}(\tau)\big)\right].$$

The expression (3.13) establishes a beautiful relation between classical and quantum mechanics. In the quantum evolution all paths contribute but they are weighted with the complex weight $\mathrm{e}^{i\mathcal{A}/\hbar}$. Therefore, paths close to solutions of the classical equations of motion, which thus leave the action stationary, give the largest contributions to the path integral, and completely dominate the integral when the action is large compared to $\hbar$.

3.3.5 Discussion

In the action (3.11), the two terms play quite different roles. The potential determines the contribution of paths as a function of the value of $\mathbf{q}(t)$ at each time, and determines the physical properties of the quantum system.

The kinetic term $\int \mathrm{d}t\, \dot{\mathbf{q}}^2$, in contrast, determines the space of paths that contribute to the integral and, thus, is essential for the very existence of the path integral. It selects paths regular enough, that is, those for which $[\mathbf{q}(t+\varepsilon)-\mathbf{q}(t)]^2/\varepsilon$ remains finite when ε goes to zero. These paths are typical of Brownian motion or random walk.

The kinetic term really belongs to the integration measure. Moreover, the explicit expression of the kinetic term, which involves $\dot{q}$, is somewhat formal since the typical paths that contribute to the path integral are continuous (they satisfy a Hölder condition of order $1/2$) but not differentiable.

However, a more mathematically correct notation would be less intuitive. In particular, it is clear in expression (3.12) that the maxima of the integrand correspond to paths that minimize the action (3.11), that is, that satisfy

$$\frac{\delta \mathcal{S}}{\delta q_i(t)} = 0 \text{ with } \frac{\delta^2 \mathcal{S}}{\delta q_i(t_1)\delta q_j(t_2)} \geq 0\,,$$

in the sense of operators. (δ denotes functional derivatives a generalization of normal derivatives, a notion defined later). They are thus solutions of the equation of the classical motion, here Euclidean (or in imaginary time), which are differentiable functions. This observation is specially relevant for $\hbar \to 0$ where classical solutions are saddle points or stationary points of the integrand in the path integral. Though only non-differentiable paths contribute to a path integral, in the semi-classical limit $\hbar \to 0$, the leading contributions come from paths close to differentiable classical paths.

3.4 Quantum partition function

We discuss now one of the simplest quantities: the quantum partition function. The potential is again assumed to be time-independent.

Trace of an operator. The trace of an operator O defined in terms of matrix elements in the position basis is given by:

$$\operatorname{tr} O = \operatorname{tr} \int \mathrm{d}q \, |q\rangle \langle q| \, O = \int \mathrm{d}q \, \operatorname{tr} \left(|q\rangle \langle q| \, O\right) = \int \mathrm{d}q \, \langle q| \, O \, |q\rangle \, , \qquad (3.14)$$

where the completeness relation (3.2) has been used.

Partition function. The quantum partition function $\mathcal{Z}(\beta) = \operatorname{tr} \mathrm{e}^{-\beta H}$ (β is the inverse temperature) has a path integral representation that follows directly from the representation of the matrix elements of the statistical operator $\mathrm{e}^{-\beta H}$. Indeed, using relation (3.14),

$$\mathcal{Z}(\beta) = \operatorname{tr} \mathrm{e}^{-\beta H} \equiv \operatorname{tr} U(\beta, 0) = \int \mathrm{d}q \, \langle \mathbf{q}| \, U(\beta, 0) \, |\mathbf{q}\rangle \, .$$

Introducing the path integral representation (3.12) of $\langle \mathbf{q}''|\, U(\beta,0)\, |\mathbf{q}'\rangle$ for $\mathbf{q}' = \mathbf{q}(0)$ and $\mathbf{q}'' = \mathbf{q}(\beta)$, one finds that the paths that contribute to the partition function satisfy the periodic boundary conditions $\mathbf{q}(0) = \mathbf{q}(\beta)$, and one integrates over all values of $\mathbf{q}(0)$. We express these conditions by the notation

$$\mathcal{Z}(\beta) = \int_{\mathbf{q}(0)=\mathbf{q}(\beta)} [\mathrm{d}q(t)] \exp\left[-\mathcal{S}(\mathbf{q})\right]. \tag{3.15}$$

These conditions define closed paths, which also correspond to the set of periodic functions $\mathbf{q}(t)$ with period β.

Low temperature limit. The ground state energy E_0 of the Hamiltonian can be derived from the partition function by studying the low temperature, $\beta \to \infty$ limit since

$$\lim_{\beta\to\infty} \frac{1}{\beta} \ln \mathcal{Z}(\beta) = -E_0 \,.$$

This remark is specially relevant when the structure of the vacuum is not trivial.

Note that in the path integral one can impose boundary conditions at $t = 0$ and $t = \beta$ as well as at $t = \pm\beta/2$ because the action is time-translation invariant. However, in the limit $\beta \to \infty$, in the first case one is led to integrate over all paths with $t \geq 0$ and an initial condition $q(0) = 0$, while in the latter case the resulting formalism is explicitly time-translation invariant since one integrates from $-\infty$ to $+\infty$. This formalism, clearly, is simpler.

3.5 Explicit calculation: Gaussian path integrals

We have defined path integrals as formal limits of integrals with discrete times. One could thus fear that any calculation of a path integral would require returning to its definition as a limit of discrete time integrals. This is fortunately not the case; most calculations make no reference to the limiting process, and this gives a practical justification to the introduction of this new mathematical entity. This will be illustrated in this section, first with the example of free motion, then with the harmonic oscillator, both corresponding to Gaussian path integrals.

3.5.1 Free motion

In the example of free motion $V \equiv 0$ (in one dimension for simplicity and with $\hbar = 1$)), the Euclidean action is the simple quadratic form in $q(t)$,

$$\mathcal{S}(q) = \int_0^\beta \tfrac{1}{2} m\dot{q}^2(t)\mathrm{d}t.$$

The corresponding path integral (3.12),

$$\langle q'' \, | U(\beta, 0) | \, q' \rangle = \int_{q(0)=q'}^{q(\beta)=q''} [\mathrm{d}q(t)] \exp \left[-\mathcal{S}(\mathbf{q}) \right],$$

is Gaussian and thus can be calculated explicitly. We first change variables, $q(t) \mapsto r(t)$, (a translation at each time t):

$$q(t) = q_c(t) + r(t),$$

where the function q_c is determined below but satisfies the boundary conditions

$$q_c(0) = q' \,, \;\; q_c(\beta) = q'' \;\; \Rightarrow \;\; r(0) = r(\beta) = 0 \,. \tag{3.16}$$

The action becomes

$$\mathcal{S}(q_c + r) = \mathcal{S}(q_c) + \mathcal{S}(r) + m \int_0^\beta \mathrm{d}t \, \dot{q}_c(t) \dot{r}(t) \,.$$

Since $r(0) = r(\beta) = 0$, the term linear in r can be written as

$$\int_{t'}^{t''} \dot{q}_c(t)\dot{r}(t)\mathrm{d}t = -\int_{t'}^{t''} \ddot{q}_c(t)r(t)\mathrm{d}t\,. \tag{3.17}$$

The linear term vanishes if the function $q_c(t)$ is a solution of the equation of the free classical motion:

$$m\ddot{q}_c(t) = 0\,.$$

The solution that satisfies the conditions (3.16) is

$$q_c(t) = q' + \frac{t}{\beta}(q'' - q').$$

One infers

$$\mathcal{S}(q_c) = \frac{m}{2\beta}(q'' - q')^2.$$

Since the change of variables is a translation, the Jacobian of the transformation is equal to 1 and $[dq(t)] = [\mathrm{d}r(t)]$. We thus obtain

$$\langle q''|\, \mathrm{e}^{-\beta\hat{p}^2/2m}\, |q'\rangle = \mathcal{N} \exp\left[-\frac{m}{2\beta}(q''-q')^2\right],$$

where

$$\mathcal{N} = \int [\mathrm{d}r(t)] \exp\left[-\frac{m}{2}\int_0^\beta \mathrm{d}t\, \dot{r}^2(t)\right]$$

with $r(0) = r(\beta) = 0$.

Since the normalization $\mathcal{N}$ does not depend on q', q'', the expression is consistent with the exact result. The path integral $\mathcal{N}$ is the value of $\langle q''|\, \mathrm{e}^{-\beta\hat{p}^2/2m}\, |q'\rangle$ for $q' = q'' = 0$. To determine it, one must either return to discrete time intervals, or use some independent information.

3.5.2 The quantum harmonic oscillator

The Hamiltonian of the one-dimensional harmonic oscillator can be written as

$$H_0 = \frac{1}{2m}\hat{p}^2 + \frac{1}{2}m\omega^2\hat{q}^2, \tag{3.18}$$

where the constant $2\pi/\omega$ is the period of the classical oscillations. The corresponding Euclidean action is

$$\mathcal{S}_0(q) = \int_0^\beta \left[\tfrac{1}{2}m\dot{q}^2(t) + \tfrac{1}{2}m\omega^2 q^2(t)\right] \mathrm{d}t\,, \tag{3.19}$$

which, again, is a quadratic form in $q(t)$. Therefore, the path integral (3.12),

$$\langle q''\, | U_0(\beta, 0) |\, q' \rangle = \int_{q(0)=q'}^{q(\beta)=q''} [\mathrm{d}q(t)]\, \mathrm{e}^{-\mathcal{S}_0(q)}, \tag{3.20}$$

remains Gaussian.

It is convenient to divide the calculation into several steps. The easiest part, and to some extent the most useful one, is the determination of the explicit dependence on the boundary conditions, that is, on q', q''.

One changes variables $q(t) \mapsto r(t)$ (a translation at each time t), setting

$$q(t) = q_c(t) + r(t),$$

where the functions $q_c(t)$ and $r(t)$ satisfy the boundary conditions (3.16) and $q_c(t)$ is determined below. The action becomes

$$\mathcal{S}_0(q_c + r) = \mathcal{S}_0(q_c) + \mathcal{S}_0(r) + m \int_0^\beta \mathrm{d}t \left(\dot{q}_c(t)\dot{r}(t) + \omega^2 q_c(t) r(t)\right).$$

One integrates by parts the term proportional to $\dot{r}\dot{q}_c$ as in equation (3.17). One then chooses the function $q_c(t)$, solution of the equation

$$-m\ddot{q}_c + m\omega^2 q_c = 0\,. \tag{3.21}$$

The term linear in $r(t)$ then cancels.

One notices that $q_c(t)$ satisfies the classical motion equation derived from the action $\mathcal{S}_0$ corresponding to a motion in an inverted harmonic potential $-\frac{1}{2}m\omega^2 q^2$ (the $-$ sign reflecting the Euclidean time).

The action (3.19) then reduces to the sum of two terms,

$$\mathcal{S}_0(q) = \mathcal{S}_0(q_c) + \mathcal{S}_0(r),$$

where $\mathcal{S}_0(q_c)$ is the classical action evaluated on the trajectory q_c. The path integral becomes (the Jacobian is 1)

$$\langle q'' |\, U_0(\beta, 0)\, | q' \rangle = \mathcal{N}(\omega, \beta)\, \mathrm{e}^{-\mathcal{S}_0(q_c)} \tag{3.22}$$

with

$$\mathcal{N}(\omega, \beta) = \int [\mathrm{d}r(t)] \exp\left[-\frac{1}{\hbar}\int_0^\beta \mathrm{d}t \left(\tfrac{1}{2}m\dot{r}^2(t) + \tfrac{1}{2}m\omega^2 r^2(t)\right)\right], \tag{3.23}$$

where the paths now satisfy the boundary conditions $r(0) = r(\beta) = 0$.

The classical action. One can write the solution of equation (3.21) as

$$q_c(t) = \frac{1}{\sinh(\omega\beta)}\left[q' \sinh\bigl(\omega(\beta - t)\bigr) + q'' \sinh\bigl(\omega t\bigr)\right].$$

In expression (3.19), an integration by parts,

$$\int \dot{q}^2 \,\mathrm{d}t = q\dot{q} - \int q\ddot{q}\,\mathrm{d}t\,,$$

combined with equation (3.21), then simplifies the calculation of the classical action $\mathcal{S}_0(q_c)$. One finds

$$\mathcal{S}_0(q_c) = \frac{m\omega}{2\sinh\omega\beta}\left[\left(q'^2 + q''^2\right)\cosh\omega\beta - 2q'q''\right].$$

Normalization. The remaining Gaussian integral (3.23) no longer depends on q', q'' and gives a simple normalization. Since, as expected, a direct calculation involves an infinite factor, for essentially pedagogical reasons, we postpone its calculation.

The complete expression is

$$\langle q''|\, U_0(\beta,0)\,|q'\rangle = \left(\frac{m\omega}{2\pi\,\sinh\omega\beta}\right)^{1/2} \mathrm{e}^{-\mathcal{S}_0(q_c)}\,.$$

By contrast, the matrix density at thermal equilibrium is independent of the normalization since

$$\langle q''|\,\rho(\beta)\,|q'\rangle = \frac{1}{\mathcal{Z}_0(\beta)}\,\langle q''|\,U_0(\beta,0)\,|q'\rangle \ \text{ with } \mathcal{Z}_0(\beta) = \operatorname{tr} U_0(\beta,0).$$

Then,

$$\mathcal{Z}_0(\beta) = \mathcal{N}\int \mathrm{d}q\, \exp\left[-m\omega\tanh(\omega\beta/2)q^2\right] = \mathcal{N}\sqrt{\frac{\pi}{m\omega\tanh(\omega\beta/2)}}$$

and thus

$$\langle q''|\,\rho(\beta)\,|q'\rangle = \frac{[m\omega\tanh(\omega\beta/2)]^{1/2}}{\pi^{1/2}}\,\mathrm{e}^{-\mathcal{S}_0(q_c)}\,.$$

3.6 Correlation functions: generating functional

In the path integral (3.15), the integrand $\mathrm{e}^{-\mathcal{S}(q)}$ defines a positive measure for paths. To this measure correspond expectation values, defined by

$$\langle \mathcal{F}(q) \rangle \equiv \frac{1}{\mathcal{Z}} \int [\mathrm{d}q(t)] \mathcal{F}(q)\, \mathrm{e}^{-\mathcal{S}(q)} \ \text{ with } \mathcal{Z} = \int [\mathrm{d}q(t)]\, \mathrm{e}^{-\mathcal{S}(q)}\,.$$

The normalization $\mathcal{Z}$ is chosen in such a way that $\langle 1 \rangle = 1$.

3.6.1 Correlation functions

Moments of the measure of the form

$$\langle q(t_1) q(t_2) \ldots q(t_n) \rangle = \mathcal{Z}^{-1} \int [\mathrm{d}q(t)] q(t_1) q(t_2) \ldots q(t_n) \exp[-\mathcal{S}(q)], \quad (3.24)$$

where $\langle \bullet \rangle$ means expectation value, are called correlation functions: a correlation function that depends on n different times is called an n-point function.

On a finite time interval β, the path integral definition requires some boundary conditions. For simplicity, we choose in most of these lectures periodic boundary conditions: $q(\beta/2) = q(-\beta/2)$. Then, the normalization $\mathcal{Z}$ is the quantum partition function.

Of course, it is possible to define correlation functions corresponding to other boundary conditions in the path integral but we will not discuss them here, all explicit expressions in the case of Gaussian integrals being more complicated.

A physical interpretation of these correlation functions will be given later. Here, they appear only as useful mathematical quantities.

3.6.2 Generating functionals

In the discussion of algebraic properties of correlation functions, generating functionals and functional derivatives provide very useful tools. We define them now.

We consider an infinite set $\{F^{(n)}(t_1, \dots, t_n)\}$, $n = 0, 1, \dots$, of symmetric functions of their arguments. We introduce an additional function $f(t)$ of one variable and the following formal series in f:

$$\mathcal{F}(f) = \sum_{n=0}^{\infty} \frac{1}{n!} \int \mathrm{d}t_1 \dots \mathrm{d}t_n \, F^{(n)}(t_1, \dots, t_n) f(t_1) \dots f(t_n).$$

The sum $\mathcal{F}(f)$ is a generating functional of the set of functions $F^{(n)}$.

In fact, more generally, we will admit for $F^{(n)}$'s also mathematical distributions (like the Dirac δ-function and its derivatives). Then, the function $f(t)$ must belong to the corresponding set of test functions and, thus, must be sufficiently differentiable.

The correlation functions that we have defined,

$$Z^{(n)}(t_1, \dots, t_n) \equiv \langle q(t_1) \dots q(t_n) \rangle \,,$$

are symmetric functions of their arguments. A generating functional of correlation functions is then

$$\begin{aligned} \mathcal{Z}(f) &= \sum_{n=0} \frac{1}{n!} \int \mathrm{d}t_1 \dots \mathrm{d}t_n \, Z^{(n)}(t_1, \dots, t_n) f(t_1) \dots f(t_n) \\ &= \sum_{n=0} \frac{1}{n!} \int \mathrm{d}t_1 \dots \mathrm{d}t_n \, \langle q(t_1) \dots q(t_n) \rangle \, f(t_1) \dots f(t_n). \end{aligned}$$

The latter series can be formally summed, by exchanging integrals and expectation value (because it is a linear operation). One finds the simple formula

$$\mathcal{Z}(f) = \left\langle \exp \left[\int \mathrm{d}t \, q(t) f(t) \right] \right\rangle . \tag{3.25}$$

3.6.3 Functional derivative

To recover the functions $F^{(n)}$ from the generating functional $\mathcal{F}(f)$, one can use functional differentiation, an operation that we now define.

Functional differentiation with respect to a function $f(t)$, which we denote by $\delta/\delta f(t)$ to distinguish it from normal derivatives, is defined by the usual algebraic properties, linearity and Leibnitz rule:

$$\begin{aligned} \frac{\delta}{\delta f(t)}\left[\mathcal{F}_1(f)+\mathcal{F}_2(f)\right] &= \frac{\delta}{\delta f(t)}\mathcal{F}_1(f)+\frac{\delta}{\delta f(t)}\mathcal{F}_2(f), \\ \frac{\delta}{\delta f(t)}\left[\mathcal{F}_1(f)\mathcal{F}_2(f)\right] &= \mathcal{F}_1(f)\frac{\delta}{\delta f(t)}\mathcal{F}_2(f)+\mathcal{F}_2(f)\frac{\delta}{\delta f(t)}\mathcal{F}_1(f) \end{aligned}$$

together with

$$\frac{\delta}{\delta f(u)}f(t)=\delta(t-u),$$

where $\delta(t)$ is Dirac's function (more accurately distribution).

For example, the first derivative of $\mathcal{F}(f)$ is

$$\frac{\delta}{\delta f(u)}\mathcal{F}(f)=\sum_{n=0}^{\infty}\frac{1}{n!}\int \mathrm{d}t_1\ldots \mathrm{d}t_n\, F^{(n+1)}(u,t_1,\ldots,t_n)f(t_1)\ldots f(t_n).$$

Differentiating now p times and setting $f\equiv 0$, one obtains

$$F^{(p)}(t_1,\ldots,t_p)=\left\{\left(\prod_{i=1}^{p}\frac{\delta}{\delta f(t_i)}\right)\mathcal{F}\right\}\Bigg|_{f\equiv 0}.$$

In the example (3.25), these identities become

$$\frac{\delta\mathcal{Z}(f)}{\delta f(t_1)}=\left\langle q(t_1)\exp\left[\int \mathrm{d}t\, q(t)f(t)\right]\right\rangle,$$

and, more generally,

$$\left(\prod_{i=1}^{p}\frac{\delta}{\delta f(t_i)}\right)\mathcal{Z}(f)=\left\langle\prod_{i=1}^{p}q(t_i)\exp\left[\int \mathrm{d}t\, q(t)f(t)\right]\right\rangle.$$

In the limit $f \equiv 0$, one thus obtains

$$\left\langle \prod_{i=1}^{p} q(t_i) \right\rangle = \left(\prod_{i=1}^{p} \frac{\delta}{\delta f(t_i)} \right) \mathcal{Z}(f) \bigg|_{f \equiv 0} .$$

Remark. This formalism also applies when the $F^{(n)}$ are not functions in the strict sense but also distributions. For example,

$$\begin{aligned} \frac{\delta}{\delta f(u)} \frac{\mathrm{d} f(t)}{\mathrm{d}t} &= \frac{\delta}{\delta f(u)} \frac{\mathrm{d}}{\mathrm{d}t} \int \mathrm{d}v \, \delta(t-v) f(v) \\ &= \frac{\mathrm{d}}{\mathrm{d}t} \delta(t-u), \end{aligned}$$

where $\delta(t)$ is Dirac's δ-function. With this extension, the classical equations of motion in the Lagrangian formalism can be obtained by functional differentiation of the action.

For example, the functional derivative of the classical action

$$\mathcal{A}(q) = \int \mathrm{d}t \left[\tfrac{1}{2} \big(\dot{q}(t)\big)^2 - V\big(q(t)\big) \right]$$

is

$$\frac{\delta \mathcal{A}}{\delta q(\tau)} = \int \mathrm{d}t \left[\dot{q}(t) \frac{\mathrm{d}}{\mathrm{d}t} \delta(t-\tau) - V'(q)\delta(t-\tau) \right] = -\ddot{q}(\tau) - V'\big(q(\tau)\big).$$

The equation of the classical motion can thus be written as

$$\frac{\delta \mathcal{A}(q)}{\delta q(\tau)} = 0\,.$$

3.7 Correlation functions and time-ordered products

We consider the n-point function

$$Z^{(n)}(t_1, t_2, \dots, t_n) = \int [\mathrm{d}q]\, q(t_1) \dots q(t_n)\, \mathrm{e}^{-\mathcal{S}(q)}, \tag{3.26}$$

with periodic boundary conditions $q(\beta/2) = q(-\beta/2$ and

$$\mathcal{S}(q) = \int_{-\infty}^{+\infty} \mathrm{d}t\ \left[\tfrac{1}{2}m\dot{q}^2(t) + V\left(q(t)\right)\right].$$

The corresponding correlation function is then

$$\langle q(t_1) \dots q(t_n) \rangle = Z^{(n)}(t_1, \dots, t_n)/\mathcal{Z}(\beta)\,,$$

where $\mathcal{Z}(\beta) = \operatorname{tr} \mathrm{e}^{-\beta H}$ is the partition function. We then order times:

$$-\beta/2 \le t_1 \le t_2 \le \dots \le t_n \le \beta/2\,. \tag{3.27}$$

We decompose the time interval $(-\beta/2, \beta/2)$ into $(n+1)$ subintervals, $(-\beta/2, t_1)$, (t_1, t_2),..., $(t_n, +\beta/2)$.

The total action is the sum of the corresponding contributions:

$$\mathcal{S}(q) = \sum_{i=1}^{n+1} \mathcal{S}(t_{i-1}, t_i) \text{ with } \mathcal{S}(\tau, \tau') = \int_{\tau}^{\tau'} \left[\tfrac{1}{2} m\dot{q}^2 + V(q)\right] \mathrm{d}t$$

and $t_0 = -\beta/2\,, t_{n+1} = +\beta/2$.

We rewrite the path integral (3.26) with the help of the identity

$$\prod_{i=1}^{n} q(t_i) = \int \prod_{i=1}^{n} \mathrm{d}q_i\, \delta\left[q(t_i) - q_i\right] q_i\,.$$

The path integral then factorizes into a product of path integrals corresponding to the different subintervals.

Returning to the very definition of the path integral (equation (3.12)), using the ordering (3.4), we see that we can rewrite the n-function as

$$Z^{(n)} = \mathrm{tr}\left[\mathrm{e}^{-\beta H}\, \mathrm{e}^{t_n H}\ \hat{q}\ \mathrm{e}^{-(t_n - t_{n-1})H}\, \hat{q} \ldots \mathrm{e}^{-(t_2 - t_1)H}\, \hat{q}\ \mathrm{e}^{-t_1 H}\right].$$

For example, for $n=1$, one obtains ($t_0=-\beta/2$, $t_2=\beta/2$, $q_0=q(\pm\beta/2)$)

$$
\begin{aligned}
Z^{(1)} &= \int \mathrm{d}q_0\,\mathrm{d}q_1\,q_1 \int_{q_0} [\mathrm{d}q]\,\mathrm{e}^{-\mathcal{S}(t_0,t_1)}\,\delta\big(q(t_1)-q_1\big)\int^{q_0}[\mathrm{d}q]\,\mathrm{e}^{-\mathcal{S}(t_1,t_2)}\\
&= \int \mathrm{d}q_0\,\mathrm{d}q_1\,q_1\,\langle q_1|\,\mathrm{e}^{-(t_1+\beta/2)H}\,|q_0\rangle\,\langle q_0|\,\mathrm{e}^{-(\beta/2-t_1)H}\,|q_1\rangle\,.
\end{aligned}
$$

Then,

$$
\int \mathrm{d}q_0\,|q_0\rangle\,\langle q_0| = \mathbf{1}\,,\qquad \int \mathrm{d}q_1\,|q_1\rangle\,q_1\,\langle q_1| = \hat{q}
$$

Therefore,

$$
\begin{aligned}
Z^{(1)} &= \mathrm{tr}\left[\mathrm{e}^{-(\beta/2-t_1)H}\,\hat{q}\,\mathrm{e}^{-(t_1+\beta/2)H}\right]\\
&= \mathrm{tr}\left[\mathrm{e}^{-\beta H}\,\mathrm{e}^{t_1 H}\,\hat{q}\,\mathrm{e}^{-t_1 H}\right].
\end{aligned}
$$

Quite generally, introducing the the Heisenberg representation in imaginary time of the operator $\hat{q}$,

$$
Q(t) = \mathrm{e}^{tH}\,\hat{q}\,\mathrm{e}^{-tH},
$$

we can rewrite $Z^{(n)}$ as

$$Z^{(n)}(t_1, t_2, \ldots, t_n) = \mathrm{tr}\left[\mathrm{e}^{-\beta H}\, Q(t_n)\ldots Q(t_1)\right]. \tag{3.28}$$

The order of the operators in the right hand side reflects the time-ordering (3.27).

We now introduce a time-ordering operator T, which to a set of time-dependent operators $A_1(t_1)$,...,$A_l(t_l)$ associates the time-ordered product (T-product) of these operators. For example, for $l = 2$,

$$\mathrm{T}\left[A_1(t_1)A_2(t_2)\right] = A_1(t_1)A_2(t_2)\theta(t_1 - t_2) + A_2(t_2)A_1(t_1)\theta(t_2 - t_1).$$

At equal times the expression is not defined if the operators then do not commute.

We can then rewrite expression (3.28), irrespective now of the order between the times $t_1, \ldots, t_n$, as

$$Z^{(n)}(t_1, t_2, \ldots, t_n) = \mathrm{tr}\left\{\mathrm{e}^{-\beta H}\, \mathrm{T}\left[Q(t_1)Q(t_2)\ldots Q(t_n)\right]\right\}. \tag{3.29}$$

Therefore,

$$\langle q(t_1)q(t_2)\dots q(t_n)\rangle = \mathcal{Z}^{-1}(\beta)\,\mathrm{tr}\left\{\mathrm{e}^{-\beta H}\,\mathrm{T}\left[Q(t_1)Q(t_2)\dots Q(t_n)\right]\right\}.$$

After continuation to real time $t_i \mapsto it_i/\hbar$, but β remaining real, $Q(t)$ becomes the usual Heisenberg representation of the operator $\hat{q}$,

$$Q(t) = \mathrm{e}^{itH}\,\hat{q}\,\mathrm{e}^{-itH}$$

and one obtains the thermal average of the n-point function at temperature $1/\beta$.

The zero temperature limit. We now assume that the Hamiltonian H has a unique normalizable ground state $|0\rangle$. In the limit $\beta \to \infty$, the statistical operator becomes a projector onto the ground state,

$$\mathrm{e}^{-\beta H} \underset{\beta\to\infty}{\sim} \mathrm{e}^{-\beta E_0} |0\rangle\langle 0|$$

and one obtains

$$\langle q(t_1)q(t_2)\dots q(t_n)\rangle = \langle 0| \mathrm{T}\,[Q(t_1)Q(t_2)\dots Q(t_n)]\,|0\rangle\,. \tag{3.30}$$

For example, for the two-point function, the relation becomes

$$\langle q(t_1)q(t_2)\rangle = \langle 0|\,\hat{q}\,\mathrm{e}^{-|t_2-t_1|(H-E_0)}\,\hat{q}\,|0\rangle\,. \tag{3.31}$$

After continuation to real time, we find a relation between the path integral and the ground state (or vacuum in the quantum field theory language) expectation value of the time ordered product of Heisenberg operators. These expectation values generate Green's functions from which one can, for instance, calculate scattering amplitudes, as we shall see later.

3.8 General Gaussian path integral and correlation functions

We now show how to derive all expectation values with a Gaussian weight, here correlation functions, from a Gaussian integral where a linear term is added to the quadratic form.

3.8.1 General Gaussian path integral

We consider the Gaussian path integral

$$\operatorname{tr} U_{\mathrm{G}}(\beta/2, -\beta/2; b) = \int [\mathrm{d}q(t)] \exp[-\mathcal{S}_{\mathrm{G}}(q, b)] \tag{3.32}$$

with periodic boundary conditions: $q(\beta/2) = q(-\beta/2)$ and

$$\begin{aligned} \mathcal{S}_{\mathrm{G}}(q, b) = \mathcal{S}_0(q) - \int_{-\beta/2}^{\beta/2} \mathrm{d}t\, b(t) q(t) \\ = \int_{-\beta/2}^{\beta/2} \mathrm{d}t \left[\tfrac{1}{2} m \dot{q}^2(t) + \tfrac{1}{2} m\omega^2 q^2(t) - b(t) q(t)\right]. \end{aligned} \tag{3.33}$$

Due to periodic boundary conditions, we can extend $q(t)$ and $b(t)$ as periodic functions of t of period β and t as a cyclic variable. This also implies time translation invariance on the circle.

Calculation. The integral, which is a functional of $b(t)$, can be calculated by first eliminating the linear term in $\mathcal{S}_{\mathrm{G}}(q,b)$.

Again, the calculation is based on a change variables, a translation of the path $q(t) \mapsto r(t)$ with

$$q(t) = q_c(t) + r(t), \quad q_c(\beta/2) = q_c(-\beta/2) \;\Rightarrow\; r(\beta/2) = r(-\beta/2), \quad (3.34)$$

where the function $q_c(t)$ is determined below. Then,

$$\mathcal{S}_{\mathrm{G}}(q,b) = \mathcal{S}_0(r) + \mathcal{S}_{\mathrm{G}}(q_c,b) + \mathcal{S}_{\mathrm{lin.}}(r,b),$$

where $\mathcal{S}_{\mathrm{lin.}}$, the linear term in r, is

$$\mathcal{S}_{\mathrm{lin.}}(r,b) = \int_{-\beta/2}^{\beta/2} \mathrm{d}t \left[m\dot{q}_c(t)\dot{r}(t) + m\omega^2 q_c(t)r(t) - b(t)r(t)\right].$$

One integrates by parts $\dot{q}_c \dot{r}$, taking into account $r(\beta/2) = r(-\beta/2)$,

$$\int_{-\beta/2}^{\beta/2} \mathrm{d}t\, \dot{q}_c(t)\dot{r}(t) = [\dot{q}_c(\beta/2) - \dot{q}_c(-\beta/2)]\, r(\beta/2) - \int_{-\beta/2}^{\beta/2} \mathrm{d}t\, \ddot{q}_c(t) r(t).$$

One obtains

$$\begin{aligned}\mathcal{S}_{\text{lin.}}(r,b) = \int_{-\beta/2}^{\beta/2} \mathrm{d}t \left[-m\ddot{q}_c(t) + m\omega^2 q_c(t) - b(t)\right] r(t) \\ + mr(\beta/2)\left[\dot{q}_c(\beta/2) - \dot{q}_c(-\beta/2)\right].\end{aligned}$$

The coefficient of the term linear in r vanishes if the function $q_c(t)$ is a solution of the classical equation of motion

$$-\ddot{q}_c(t) + \omega^2 q_c(t) = b(t)/m$$

and satisfies $\dot{q}_c(\beta/2) = \dot{q}_c(-\beta/2)$ (in addition to $q_c(\beta/2) = q_c(-\beta/2)$).

The solution can be written as (time translation invariance is used)

$$q_c(t) = \frac{1}{m} \int_{-\beta/2}^{\beta/2} \Delta(t-u) b(u) \mathrm{d}u \,. \tag{3.35}$$

The function $\Delta(t)$ is the solution of the equation ($\delta(t)$ is Dirac's function)

$$-\ddot{\Delta}(t) + \omega^2 \Delta(t) = \delta(t) \tag{3.36}$$

with the periodic boundary conditions, $\Delta(\beta/2) = \Delta(-\beta/2)$, $\dot{\Delta}(\beta/2) = \dot{\Delta}(-\beta/2)$. One finds

$$\Delta(t) = \frac{1}{2\omega \, \sinh(\omega\beta/2)} \cosh\big(\omega(\beta/2 - |t|)\big). \tag{3.37}$$

To verify the result directly one needs the relations between distributions,

$$\frac{\mathrm{d}}{\mathrm{d}t}|t| = \mathrm{sgn}(t), \quad \frac{\mathrm{d}}{\mathrm{d}t}\,\mathrm{sgn}(t) = 2\delta(t),$$

where $\mathrm{sgn}(t)$ is the sign function, $\mathrm{sgn}(t) = 1$ for $t > 0$, $\mathrm{sgn}(t) = -1$ for $t < 0$.

The function $\Delta(t)$, which plays an essential role in perturbative expansions around the harmonic oscillator, is also called propagator. Its limit when $\beta \to \infty$ (assuming $\omega > 0$) is the solution that decreases at infinity,

$$\Delta(t) = \frac{1}{2\omega}\,\mathrm{e}^{-\omega|t|} = \frac{1}{2\pi}\int_{-\infty}^{+\infty} \mathrm{d}\kappa \frac{\mathrm{e}^{i\kappa t}}{\kappa^2 + \omega^2}\,. \tag{3.38}$$

Note that the kernel $\Delta(t)$ has no $\omega = 0$ limit.

The kernel $\Delta(t_1 - t_2)$ is the inverse of the differential operator $-\mathrm{d}_t^2 + \omega^2$ with periodic boundary conditions. It depends only on the difference $t_2 - t_1$ because periodic boundary conditions are time-translation invariant. We have already pointed out that the interval $[-\beta/2, \beta/2]$ can be identified with a circle and time with an angular variable.

3.8.2 Remark

A general remark simplifies the calculation of the classical action. One calculates the action corresponding to $\lambda q_c(t)$:

$$\mathcal{S}_{\rm G}(\lambda q_c, b) = \int_{-\beta/2}^{\beta/2} \mathrm{d}t \left\{\lambda^2 \left[\tfrac{1}{2}m\dot{q}_c^2(t) + \tfrac{1}{2}m\omega^2 q_c^2(t)\right] - \lambda b(t) q_c(t)\right\}.$$

Since q_c is a solution of the classical equation, the action $\mathcal{S}_{\rm G}(\lambda q_c, b)$ is stationary at the solution, that is for $\lambda = 1$:

$$\frac{\mathrm{d}}{\mathrm{d}\lambda}\mathcal{S}_{\rm G}(\lambda q_c, b)\bigg|_{\lambda=1} = 0\,.$$

One infers

$$\int_{-\beta/2}^{\beta/2} \mathrm{d}t \left[\tfrac{1}{2}m\dot{q}_c^2(t) + \tfrac{1}{2}m\omega^2 q_c^2(t)\right] = \frac{1}{2}\int_{-\beta/2}^{\beta/2} \mathrm{d}t\, b(t) q_c(t).$$

Thus,

$$\mathcal{S}_{\mathrm{G}}(q_c, b) = -\frac{1}{2}\int_{-\beta/2}^{\beta/2} \mathrm{d}t\, q_c(t)b(t) = -\frac{1}{2m}\int_B \mathrm{d}t\,\mathrm{d}u\, b(t)\Delta(t-u)b(u)$$

with $B \equiv t, u \in [-\beta/2, \beta/2]$.

The remaining integration over the path $r(t)$ yields a normalization that is identical to the partition function of the harmonic oscillator, $\mathcal{Z}_0(\beta) = \mathrm{tr}\, \mathrm{e}^{-\beta H_0}$ (H_0 is the Hamiltonian of the harmonic oscillator). The final expression is

$$\begin{aligned} \mathcal{Z}_{\mathrm{G}}(\beta, b) &= \mathrm{tr}\, U_{\mathrm{G}}(\beta/2, -\beta/2; b) = \mathcal{Z}_0(\beta)\, \mathrm{e}^{-\mathcal{S}_{\mathrm{G}}(q_c, b)} \\ &= \mathcal{Z}_0(\beta) \exp\left[\frac{1}{2m}\int_B \mathrm{d}u\,\mathrm{d}v\, b(v)\Delta(v-u)b(u)\right]. \end{aligned} \tag{3.39}$$

3.8.3 Gaussian correlation functions. Wick's theorem

We now introduce Gaussian expectation values, which we denote by $\langle \bullet \rangle_0$, corresponding to the normalized Gaussian distribution $\mathrm{e}^{-\mathcal{S}_0} / \mathcal{Z}_0(\beta)$ with periodic boundary conditions.

The functional (3.32), divided by the partition function $\mathcal{Z}_0(\beta)$ which can then be written as

$$\mathcal{Z}_{\mathrm{G}}(\beta, b)\mathcal{Z}_0^{-1}(\beta) = \left\langle \exp\left[\int_{-\beta/2}^{\beta/2} \mathrm{d}t\, b(t)q(t)\right]\right\rangle_0 ,$$

generates the corresponding correlation functions (equation (3.25)). Acting by functional differentiation (functional derivatives have been defined in section 3.6.3) on both sides, in the limit $b \equiv 0$ one obtains

$$\mathcal{Z}_0^{-1}(\beta) \left[\prod_{j=1}^{\ell} \frac{\delta}{\delta b(t_j)}\right] \mathcal{Z}_{\mathrm{G}}(\beta, b)\bigg|_{b\equiv 0} = \langle q(t_1)q(t_2)\ldots q(t_\ell)\rangle_0 . \qquad (3.40)$$

Replacing $\mathcal{Z}_{\mathrm{G}}(b,\beta)$ by the explicit result (3.39) in the left hand side of equation (3.40), one then finds

$$\langle q(t_1)\dots q(t_\ell)\rangle_0 = \prod_{j=1}^{\ell} \frac{\delta}{\delta b(t_j)} \exp\left[\frac{1}{2m}\int \mathrm{d}u\,\mathrm{d}v\, b(v)\Delta(v-u)b(u)\right]\bigg|_{b\equiv 0}. \tag{3.41}$$

In particular, the second derivative yields the two-point correlation function

$$\langle q(t)q(u)\rangle_0 = \mathcal{Z}_0^{-1}(\beta)\,\frac{\delta^2}{\delta b(t)\delta b(u)}\mathcal{Z}_{\mathrm{G}}(\beta,b)\bigg|_{b\equiv 0} = \frac{1}{m}\Delta(t-u). \tag{3.42}$$

Wick's theorem. Quite generally, each functional differentiation of the expression (3.41) generates a factor b:

$$\begin{aligned}&\frac{\delta}{\delta b(t_1)}\exp\left[\frac{1}{2m}\int \mathrm{d}u\,\mathrm{d}v\, b(v)\Delta(v-u)b(u)\right]\\ &\quad = \frac{1}{m}\int \mathrm{d}u_1\,\Delta(t_1-u_1)b(u_1)\exp\left[\frac{1}{2m}\int \mathrm{d}u\,\mathrm{d}v\, b(v)\Delta(v-u)b(u)\right].\end{aligned}$$

In the limit $b \equiv 0$, the only surviving terms correspond to pairings of functional differentiations. We find a characteristic property of the centred Gaussian measure: all correlation functions can be expressed in terms of the two-point function in a form expressed by Wick's theorem:

$$\begin{aligned}\langle q(t_1)q(t_2)\dots q(t_\ell)\rangle_0 &= \sum_{P\{1,2,\dots,\ell\}} \frac{1}{m^\ell}\Delta(t_{P_1}-t_{P_2})\dots\Delta(t_{P_{\ell-1}}-t_{P_\ell}) \\ &= \sum_{P\{1,2,\dots,\ell\}} \langle q(t_{P_1})q(t_{P_2})\rangle_0 \cdots \langle q(t_{P_{\ell-1}})q(t_{P_\ell})\rangle_0 \,, \end{aligned} \tag{3.43}$$

where $P\{1,2,\dots,\ell\}$ are all possible (unordered) pairings of $\{1,2,\dots,\ell\}$. For example,

$$\begin{aligned}\langle q(t_1)q(t_2)q(t_3)q(t_4)\rangle = \langle q(t_1)q(t_2)\rangle\langle q(t_3)q(t_4)\rangle + \langle q(t_1)q(t_3)\rangle\langle q(t_2)q(t_4)\rangle \\ + \langle q(t_1)q(t_4)\rangle\langle q(t_3)q(t_2)\rangle.\end{aligned}$$

Regularity of generic paths revisited. The preceding results allow calculating the expectation value of the quantity

$$\left\langle \left(q(t+\varepsilon)-q(t)\right)^2 \right\rangle_0 = \frac{2}{m}\left[\Delta(0)-\Delta(\varepsilon)\right].$$

For $\varepsilon \to 0$, one finds

$$\left\langle \left(q(t+\varepsilon)-q(t)\right)^2 \right\rangle_0 \sim |\varepsilon|\frac{1}{m}\,. \tag{3.44}$$

This result confirms that generic trajectories contributing to the path integral are not differentiable (though continuous), and that the behaviour of $q(t+\varepsilon)-q(t)$ for $\varepsilon \to 0$ does not depend on the potential but only on the kinetic term in the action. It also implies that the average action $\langle \mathcal{S}(q) \rangle_0$ is infinite, because the kinetic term diverges.

3.9 Quantum harmonic oscillator: the partition function

As an exercise, we can now complete the calculation of the partition function $\mathcal{Z}_0(\beta)$ of the harmonic oscillator, which appears in the normalization of correlation functions in equations (3.24).

For this purpose, we use the important property that while the partition function, which is just a normalization, is not an observable, its logarithmic derivatives with respect to any parameter, are. Indeed, if σ is such a parameter,

$$\frac{\partial}{\partial\sigma}\mathcal{Z}_0(\beta) = -\int [\mathrm{d}q]\, \mathrm{e}^{-\mathcal{S}_0(q)}\, \frac{\partial \mathcal{S}_0}{\partial\sigma}.$$

Dividing both sides by $\mathcal{Z}_0(\beta)$, we obtain

$$\frac{\partial}{\partial\sigma}\ln \mathcal{Z}_0(\beta) = -\left\langle \frac{\partial \mathcal{S}_0}{\partial\sigma} \right\rangle_0.$$

Quite generally, the quantity $W = \ln \mathcal{Z}$ is called the free energy in the context of statistical physics and will play an important role later.

We now determine the dependence of the partition function on the parameter ω. Differentiating the path integral (3.20) with boundary conditions (3.15), one obtains

$$\frac{\partial}{\partial\omega}\ln\mathcal{Z}_0(\beta) = -\left\langle\frac{\partial\mathcal{S}_0}{\partial\omega}\right\rangle_0 = -m\omega\int_{-\beta/2}^{\beta/2}\mathrm{d}t\,\left\langle q^2(t)\right\rangle_0\,,$$

where $\langle\bullet\rangle_0$ stands for Gaussian expectation value with the weight $\mathrm{e}^{-\mathcal{S}_0(q)}/\mathcal{Z}_0$. Thus,

$$\frac{\partial}{\partial\omega}\ln\mathcal{Z}_0(\beta) = -\beta\omega\Delta(0) = -\frac{\beta}{2}\frac{\cosh(\omega\beta/2)}{\sinh(\omega\beta/2)}, \tag{3.45}$$

where the explicit form (3.37) of $\Delta(t)$ has been used. We infer

$$\mathcal{Z}_0(\beta) = \mathcal{N}'\frac{1}{\sinh(\beta\omega/2)}\,.$$

The constant $\mathcal{N}'$ is a pure number. Since in the limit $\beta\to\infty$, $\mathcal{Z}_0 \sim \mathrm{e}^{-\beta E_{)}}$, one concludes $\mathcal{N}' = \frac{1}{2}$. This then yields the exact partition function.

3.10 Perturbed harmonic oscillator

We now consider a potential that is the sum of a harmonic potential and a perturbation. The Hamiltonian can be written as

$$H = \frac{1}{2m} p^2 + \frac{m}{2} \omega^2 q^2 + V_\mathrm{I}(q). \tag{3.46}$$

We assume that the perturbation is a polynomial in the variable q:

$$V_\mathrm{I}(q) = \sum_{n=1} v_n q^n .$$

The corresponding partition function is given by (we still set $\hbar = 1$)

$$\mathcal{Z}(\beta) = \int [\mathrm{d}q] \exp \left\{ - \int_{-\beta/2}^{\beta/2} \left[\tfrac{1}{2} m \dot{q}^2(t) + \tfrac{1}{2} m \omega^2 q^2(t) + V_\mathrm{I}\big(q(t)\big) \right] \mathrm{d}t \right\} \tag{3.47}$$

with $q(-\beta/2) = q(\beta/2)$.

3.10.1 Perturbative expansion

The integrand (3.47) can be expanded in powers of $V_{\mathrm{I}}(q)$ and this leads to

$$\frac{\mathcal{Z}(\beta)}{\mathcal{Z}_0(\beta)} = \sum_{k=0} \frac{(-1)^k}{k!} \left\langle \left[\int \mathrm{d}t\, V_{\mathrm{I}}\big(q(t)\big)\right]^k \right\rangle_0$$

$$= \sum_{k=0} \frac{(-1)^k}{k!} \int \mathrm{d}t_1 \mathrm{d}t_2 \ldots \mathrm{d}t_k \left\langle V_{\mathrm{I}}\big(q(t_1)\big) \ldots V_{\mathrm{I}}\big(q(t_k)\big)\right\rangle_0 ,$$

where $\langle \bullet \rangle_0$ means expectation value with respect to the Gaussian measure $\mathrm{e}^{-\mathcal{S}_0}/\mathcal{Z}_0$ (equation (3.40)) with periodic boundary conditions.

Since $V_{\mathrm{I}}(q)$ is a polynomial, successive terms in the expansion can be calculated using Wick's theorem in the form (3.43). This is the basis of perturbation theory.

3.10.2 Perturbative expansion and the minimum of the potential

To each decomposition of the potential into a sum of a quadratic term and a remainder $V_{\mathrm{I}}(q)$ is associated a perturbative expansion. However, the integrand is the largest in the vicinity of the paths that minimize the action. Clearly, periodic functions that minimize the action are constant functions $q(t) \equiv q_0$, to minimize the kinetic term, where the value q_0 must minimize the potential $V(q)$ and thus

$$V'(q_0) = 0\,,\ V''(q_0) > 0\,.$$

Therefore, the optimal decomposition is

$$V(q) = V(q_0) + \tfrac{1}{2} V''(q_0)\,(q - q_0)^2 + V_{\mathrm{I}}(q).$$

Specific problems associated with a degeneracy of the minimum of the potential will be discussed somewhere else.

3.10.3 Perturbative expansion in powers of $\hbar$ and steepest descent method

In this section, we reinstate Planck's constant $\hbar$ and consider the Euclidean or imaginary time action. For example, the partition function takes the form

$$\mathcal{Z} = \int_{q(-\tau/2)=q(\tau/2)} [\mathrm{d}q(t)] \exp\left[-\mathcal{S}(q)/\hbar\right],$$

where $\tau = \hbar\beta$ will be considered fixed when $\hbar \to 0$. We consider a general Hamiltonian of the form

$$H = \frac{1}{2m}p^2 + V(q),$$

where the potential $V(q)$ is expandable in powers of q (and not only a polynomial) with a unique minimum at $q = 0$ such that

$$V(q) = \tfrac{1}{2}m\omega^2 q^2 + V_{\mathrm{I}}(q), \quad V_{\mathrm{I}}(q) = O(q^3).$$

We have already discussed perturbative calculations of the partition function in the form of expansions in powers of some polynomial perturbation $V_{\mathrm{I}}(q)$. We have pointed out that an optimal harmonic approximation is provided by a quadratic approximation of the potential around its minimum.

A perturbative expansion around this harmonic approximation can be reorganized in a simple way as an expansion in powers of $\hbar$. The latter expansion differs from the simple perturbative expansion as soon as the perturbation V_{I} is no longer a monomial.

An expansion in powers of $\hbar$ can be called semi-classical but, in fact, it is the expansion in $\hbar$ based on the representation of the quantum partition function that corresponds better to the idea of a semi-classical approach.

We consider an Euclidean action $\mathcal{S}(q)$ of the form

$$\mathcal{S}(q) = \int_{-\tau/2}^{\tau/2} \left[\tfrac{1}{2} m \dot{q}^2(t) + V\bigl(q(t)\bigr)\right] \mathrm{d}t\,.$$

We evaluate the path integral in the formal limit $\hbar \to 0$, with τ fixed.

From a semi-classical viewpoint, this limit corresponds indeed to $\hbar \to 0$, but simultaneously $\beta = \tau/\hbar \to \infty$, that is, in a correlated way the temperature goes to zero, a limit that enhances small oscillations around the classical minimum and excitations close to the quantum ground state.

In this limit, the path integral has exactly a form that justifies using the steepest descent method. Since $q = 0$ corresponds to an absolute and non-degenerate minimum of the potential V, the path integral is dominated for $\hbar \to 0$ by the trivial saddle point $q(t) \equiv 0$, which minimizes both the potential and the kinetic term. The change of variables $q(t) \mapsto \sqrt{\hbar} q(t)$ in the path integral, allows a direct identification of the leading terms in the action. After the change,

$$\mathcal{S}(q)/\hbar = \frac{m}{2} \int_{-\tau/2}^{\tau/2} \left[\dot{q}^2(t) + \omega^2 q^2(t)\right] + \frac{1}{\hbar} \int_{-\tau/2}^{\tau/2} \mathrm{d}t \, V_{\mathrm{I}}\big(q(t)\sqrt{\hbar}\big).$$

Since $V_{\mathrm{I}}(q\sqrt{\hbar})/\hbar$ is at least of order $\sqrt{\hbar}$, at leading order one recovers the partition function of a harmonic oscillator.

At higher orders, the integral can be calculated by first expanding the integrand in powers of V_{I} and then collecting terms with the same powers of $\hbar$.

For any potential expandable in powers of q and at any finite order in $\hbar$, the integrand remains the product of a Gaussian factor by a polynomial in q since the terms of degree q^n in the potential start contributing only at order $\hbar^{n/2-1}$. Therefore, for any expandable potential, the expansion of $\mathcal{Z}(\tau/\hbar)$ in powers of $\hbar$ relies on Gaussian expectation values of polynomials, which can be calculated with the help of Wick's theorem.

3.11 Quantum evolution and Scattering matrix

In the preceding lectures, we have mainly discussed quantum statistical operators, and thus, formally, evolution in imaginary or euclidean time. Here, we give a few elements of real-time evolution.

Scattering S-matrix elements, quantities relevant to microscopic physics, are related to the quantum evolution operator in real time.

Therefore, we first derive the path integral representation of the evolution operator and the S-matrix in non-relativistic quantum mechanics. To illustrate the power of the formalism, we show how the perturbative expansion of the scattering amplitude, as generated by the Lippman–Schwinger's equation, can be recovered.

3.11.1 Quantum evolution and Scattering matrix

Evolution in quantum mechanics is associated with an operator acting linearly on the Hilbert space of states. Conservation of probabilities for an isolated system implies that the evolution operator must be unitary. Finally, one assumes that the evolution of an isolated system is Markovian (without memory effects). Then the evolution operator $U(t'', t')$ from time t' to time t'' satisfies the relation

$$U(t_3, t_2)U(t_2, t_1) = U(t_3, t_1).$$

Assuming the evolution differentiable, we expand $U(t+\varepsilon, t)$ for an infinitesimal time interval ε:

$$U(t+\varepsilon, t) = \mathbf{1} - i\varepsilon H(t)/\hbar + O(\varepsilon^2)\,,$$

where $H(t)$ is the quantum Hamiltonian. Equation (3.4) then implies

$$i\hbar \frac{\partial U}{\partial t}(t, t') = H(t)Ut, t'), \quad U(t', t') = \mathbf{1}\,.$$

When the operator $H(t)$ is time-independent, $U(t'',t') = U(t''-t') = \mathrm{e}^{-i(t''-t')H/\hbar}$. The evolution operators $U(t)$ then form a representation of the symmetry group of time translations. The generator of the Lie algebra $\partial/\partial t$ is represented by the operator $-iH/\hbar$.

The S-matrix. The scattering S-matrix is obtained by comparing the quantum evolution with the free evolution in the absence of interactions. More precisely, the S-matrix can be defined as the limit of the evolution operator in the so-called interaction representation:

$$S = \lim_{\substack{t'\to-\infty \\ t''\to+\infty}} \mathrm{e}^{iH_0 t''/\hbar}\, U(t'',t')\, \mathrm{e}^{-iH_0 t'/\hbar}, \tag{3.48}$$

where the Hamiltonian H_0 is the free Hamiltonian corresponding to H: its eigenstates are the free or asymptotic states at large time of quantum evolution.

3.11.2 Scattering matrix in quantum particle mechanics

In the simple quantum mechanics of a particle in a potential, examples of free and interacting Hamiltonians are simply

$$H_0 = \mathbf{p}^2/2m, \qquad H = \mathbf{p}^2/2m + V(\mathbf{q}, t). \tag{3.49}$$

The large time limit and, therefore, the S-matrix exist only if the potential decreases fast enough at large distance, or large time in such a way that for $|t| \to \infty$ the evolution converges fast enough toward the free evolution corresponding to H_0.

The matrix elements of the free evolution operator $U_0 = \mathrm{e}^{-i(t''-t')H_0/\hbar}$, corresponding to the Hamiltonian H_0 in (3.49), in d space dimensions, is given by

$$\langle \mathbf{q}''| \, U_0(t'', t') \, |\mathbf{q}'\rangle = \left(\frac{m}{2i\pi\hbar(t''-t')}\right)^{d/2} \exp\left[\frac{i}{\hbar} \frac{m\,(\mathbf{q}''-\mathbf{q}')^2}{2(t''-t')}\right].$$

In the momentum basis, the relation (3.48) between the S-matrix and the evolution operator takes the form

$$\langle \tilde{\mathbf{p}}''| \, S \, |\tilde{\mathbf{p}}'\rangle = \lim_{\substack{t'\to-\infty \\ t''\to+\infty}} \mathrm{e}^{iE''t''/\hbar} \langle \tilde{\mathbf{p}}''| \, U(t'',t') \, |\tilde{\mathbf{p}}'\rangle \, \mathrm{e}^{-iE't'/\hbar} \tag{3.50}$$

with $E' = E(\mathbf{p}'), \quad E'' = E(\mathbf{p}''), \qquad E(\mathbf{p}) = \mathbf{p}^2/2m.$

The limits $t' \to -\infty$, $t'' \to +\infty$ have to be understood mathematically in the sense of distributions (one should use test functions in the form of wave packets).

The S-matrix in the momentum basis is in general parametrized in terms of the scattering matrix $\mathcal{T}$:

$$S = 1 - i\mathcal{T}, \; \Rightarrow \; \langle \tilde{\mathbf{p}}'' \, |S| \, \tilde{\mathbf{p}}'\rangle = (2\pi\hbar)^d \delta^{(d)}(\mathbf{p}'' - \mathbf{p}') - i \, \langle \tilde{\mathbf{p}}'' \, |\mathcal{T}| \, \tilde{\mathbf{p}}'\rangle \, . \tag{3.51}$$

When the potential is time-independent, energy is conserved and one can write

$$\langle \tilde{\mathbf{p}}'' \, |\mathcal{T}| \, \tilde{\mathbf{p}}'\rangle = -2\pi\delta(E'' - E')T(\mathbf{p}'', \mathbf{p}'). \tag{3.52}$$

3.12 Path integral representation: Evolution and S-matrix

The matrix elements of the evolution operator, corresponding to a Hamiltonian of the form

$$H = p^2/2m + V(q,t),$$

are given by the path integral (expression (3.13))

$$\langle q''| \, U(t'',t') \, |q'\rangle = \int_{q(t')=q'}^{q(t'')=q''} [\mathrm{d}q(t)] \exp\left[i\mathcal{A}(q)/\hbar\right]$$

with

$$\mathcal{A}(q) = \int_{t'}^{t''} \mathrm{d}t \left[\tfrac{1}{2}m\dot{q}^2(t) - V\big(q(t),t\big)\right].$$

Phase space formulation. In the real time formulation, the path integral over phase space is replaced by

$$\langle q''|\, U(t'',t')\, |q'\rangle = \int [\mathrm{d}p(t)\mathrm{d}q(t)] \exp\left[i\mathcal{A}(p,q)/\hbar\right]. \tag{3.53}$$

The quantity $\mathcal{A}(p,q)$, which replaces the Euclidean action in the path integral, is again the classical action in the Hamiltonian formalism:

$$\mathcal{A}(p,q) = \int_{t'}^{t''} \left[p(t)\dot{q}(t) - H\big(p(t),q(t),t\big)\right] \mathrm{d}t\,.$$

Even in this more general situation the quantum evolution is obtained by summing over all paths weighted with the complex weight $\mathrm{e}^{i\mathcal{A}/\hbar}$, where $\mathcal{A}$ is the classical action in the phase space formalism.

3.12.1 Path integral and S-Matrix

We now show that the representation (3.13) of the evolution operator leads to a path integral representation for elements of the scattering S-matrix, which is particularly well suited to the study of the semi-classical limit.

The elements of the S-matrix between two wave packets are given by

$$\langle\psi_2|\, S\, |\psi_1\rangle = \lim_{\substack{t'\to-\infty \\ t''\to+\infty}} \int \mathrm{d}q'\mathrm{d}q''\, \langle\psi_2|\, \mathrm{e}^{iH_0 t''/\hbar}\, |\mathbf{q}''\rangle\, \langle\mathbf{q}''|\, U(t'',t')\, |\mathbf{q}'\rangle \times \langle\mathbf{q}'|\, \mathrm{e}^{-iH_0 t'/\hbar}\, |\psi_1\rangle\,. \tag{3.54}$$

Introducing the two wave functions $\tilde{\psi}_1(\mathbf{p})$ and $\tilde{\psi}_2(\mathbf{p})$ in the momentum basis, we define $(i = 1, 2)$

$$\psi_i(\mathbf{q},t) = \langle\mathbf{q}|\, \mathrm{e}^{-iH_0 t/\hbar}\, |\psi_i\rangle = \int \frac{\mathrm{d}^d p}{(2\pi)^d} \tilde{\psi}_i(\mathbf{p}) \exp\left[i\left(\mathbf{p}\cdot\mathbf{q} - t\frac{\mathbf{p}^2}{2m}\right)/\hbar\right]. \tag{3.55}$$

When t becomes large, the phase in expression (3.55) varies rapidly, and the integral is then dominated by the stationary points of the phase:

$$\frac{\partial}{\partial \mathbf{p}}\left(\mathbf{p}\cdot\mathbf{q}-t\frac{\mathbf{p}^2}{2m}\right)=0 \quad\Longrightarrow\quad \mathbf{q}=t\frac{\mathbf{p}}{m}\,.$$

The evaluation of the integral (3.55) thus yields the estimate

$$\psi_1(\mathbf{q},t)\underset{|t|\to\infty}{\sim}\tilde{\psi}_1(\mathbf{p})\frac{1}{(2\pi)^{d/2}}\left(\frac{m\hbar}{|t|}\right)^{d/2}\exp\left(\frac{i\pi}{4}\operatorname{sgn}t+it\frac{\mathbf{p}^2}{2m\hbar}\right)$$

with $\mathbf{p}=m\mathbf{q}/t$. We then change variables in integral (3.54), setting

$$\mathbf{q}'=\frac{t'}{m}\mathbf{p}',\qquad \mathbf{q}''=\frac{t''}{m}\mathbf{p}'',$$

and obtain

$$\begin{aligned}\langle\psi_2|\,S\,|\psi_1\rangle \propto \lim_{\substack{t'\to-\infty\\ t''\to+\infty}}\int \mathrm{d}p'\mathrm{d}p''\,\tilde{\psi}_2^*(\mathbf{p}'')\tilde{\psi}_1(\mathbf{p}')\exp\left[\frac{i}{\hbar}\left(t''\frac{\mathbf{p}''^2}{2m}-t'\frac{\mathbf{p}'^2}{2m}\right)\right]\\ \times\langle t''\mathbf{p}''/m|\,U(t'',t')\,|t'\mathbf{p}'/m\rangle\,. \end{aligned}\tag{3.56}$$

In the equation, we introduce the path integral representation (3.13) of the evolution operator:

$$\langle t''\mathbf{p}''/m|\, U(t'',t')\,|t'\mathbf{p}'/m\rangle = \int_{q(t')=t'p'/m}^{q(t'')=t''p''/m} [\mathrm{d}q(t)]\exp\bigl(i\mathcal{A}(q)/\hbar\bigr).$$

We conclude that the S-matrix can be derived from the calculation of the path integral with classical scattering boundary conditions, that is, by summing over paths solutions at large time of the free classical equations of motion.

In particular, if we know how to solve the classical equations of motion with such boundary conditions we can calculate the evolution operator and thus the S-matrix for $\hbar$ small. This leads to semi-classical approximations of the S-matrix.

3.12.2 Path integral and S-Matrix: perturbation theory.

We now show how the path integral representing the evolution operator can be calculated in the form of an expansion in powers of the potential. The path integral formalism actually organizes the perturbative expansion in a way similar to the operator formalism. From the expansion of the evolution operator we then derive the expansion of the elements of the S-matrix.

Warning. This part is quite technical, though straightforward, and requires a careful reading.

We consider a time-independent Hamiltonian

$$H = p^2/2m + V(x)$$

(setting for convenience $\hbar = 1$). The classical actions corresponding to the free Hamiltonian H_0 and to H, respectively, are

$$\mathcal{A}_0(x) = \int_{t'}^{t''} \frac{1}{2} m\dot{x}^2(t)\mathrm{d}t\,, \quad \mathcal{A}(x) = \int_{t'}^{t''} \left[\tfrac{1}{2} m\dot{x}^2(t) - V\big(x(t)\big)\right] \mathrm{d}t\,.$$

We now expand the path integral (3.13) in powers of V:

$$\langle x''|U(t'',t')|x'\rangle = \int_{x(t')=x'}^{x(t'')=x''} [\mathrm{d}x(t)]\exp\left[i\mathcal{A}(x)\right] = \sum_\ell \langle x''|U^{(\ell)}(t'',t')|x'\rangle ,$$
$$\langle x''|U^{(\ell)}(t'',t')|x'\rangle = \int_{x(t')=x'}^{x(t'')=x''} [\mathrm{d}x(t)]\,\mathrm{e}^{i\mathcal{A}_0(x)}\frac{(-i)^\ell}{\ell!}\left[\int_{t'}^{t''} V\big(x(t)\big)\mathrm{d}t\right]^\ell .$$

Since the potential must vanish at large distances, it makes sense to assume that it has a Fourier representation:

$$V(x) = (2\pi)^{-d}\int \mathrm{d}^d k\ \mathrm{e}^{ikx}\ \tilde{V}(k). \tag{3.57}$$

Introducing the representation (3.57) in the path integral,

$$\langle x''|\,U^{(\ell)}(t'',t')\,|x'\rangle = \frac{(-i)^\ell}{\ell!}\int_{t'}^{t''}\prod_j \mathrm{d}\tau_j \int \prod_{j=1}^{\ell} \tilde{V}(k_j)\frac{\mathrm{d}^d k_j}{(2\pi)^d}$$
$$\times \int_{x(t')=x'}^{x(t'')=x''}[\mathrm{d}x(t)]\exp i\left[\int_{t'}^{t''}\tfrac{1}{2}m\dot{x}^2(t)\mathrm{d}t + \sum_j k_j x(\tau_j)\right],$$

we see that each term in the perturbative expansion then involves only the calculation of a Gaussian path integral. The integrand is symmetric in the times $\tau_1,\tau_2,\ldots,\tau_\ell$. Therefore, we can order them as $t''\ge\tau_\ell\ge\tau_{\ell-1}\cdots\ge\tau_1\ge t'$ and suppress the factor $1/\ell!$.

The term of order zero in V yields a contribution $(2\pi)^d\delta(p''-p')$ to the S-matrix.

To calculate the general term explicitly, we introduce δ-functions:

$$\exp[ik_j x(\tau_j)] = \int \mathrm{d}^d x_j\,\delta\big(x_j - x(\tau_j)\big)\exp\left(ik_j x_j\right).$$

Then, in each interval $\tau_j \le t \le \tau_{j+1}$, we recognize the matrix elements of the free evolution operator (see also section 3.7), which we write in the Fourier representation.

We calculate the Fourier transform with respect to x' and x'', calling p' and p'', respectively, the corresponding momenta. We find

$$\langle \tilde{p}'' | \, U^{(\ell)}(t'', t') \, | \tilde{p}' \rangle = (-i)^{\ell} \int \prod_{j=1}^{\ell} \mathrm{d}\tau_j \tilde{V}(k_j) \frac{\mathrm{d}^d k_j}{(2\pi)^d} \mathrm{d}^d x_j \prod_{j=2}^{\ell} \frac{\mathrm{d}^d p_j}{(2\pi)^d}$$

$$\times \exp\left[\sum_{j=1}^{\ell+1} -i p_j^2 (\tau_j - \tau_{j-1})/2m + i p_j (x_j - x_{j-1}) + i k_j x_j \right]$$

with the conventions

$$\tau_0 = t', \quad \tau_{\ell+1} = t'', \quad p_{\ell+1} = p'', \quad p_1 = p', \quad x_0 = x_{\ell+1} = 0 \, .$$

The integration over the variables x_j yields δ-functions which determine the variables k_j as $k_j = p_{j+1} - p_j$.

After factorization of the free evolution operator on both sides, the limits $t'' \to +\infty$, $t' \to -\infty$ can be taken.
The corresponding S-matrix elements follow:

$$\langle \tilde{p}''|\, S^{(\ell)}\, |\tilde{p}'\rangle = (-i)^\ell \int \prod_{j=1}^{\ell} \mathrm{d}\tau_j \prod_{j=2}^{\ell} \frac{\mathrm{d}^d p_j}{(2\pi)^d}\, \mathrm{e}^{ip''^2\tau_\ell/2m}\, \tilde{V}(p'' - p_\ell)$$
$$\times\, \mathrm{e}^{ip_\ell^2(\tau_{\ell-1}-\tau_\ell)/2m} \ldots \times \mathrm{e}^{ip_2^2(\tau_1-\tau_2)/2m}\, \tilde{V}(p_2 - p')\, \mathrm{e}^{-ip'^2\tau_1/2m}\,. \quad (3.58)$$

We still have to integrate over the times τ_j. We set

$$\tau_{j+1} = \tau_j + u_j\,, \quad u_j \geq 0\,.$$

The remaining integral over τ_1 yields a δ-function of energy conservation: $2\pi\delta(E'' - E')$, which follows from time translation invariance. The integrals over the variables u_j on the positive axis yield mathematical distributions:

$$\int_0^{+\infty} \mathrm{d}u_j\, \mathrm{e}^{i(E''-E(p_j))u_j} = \frac{i}{E'' - E(p_j) + i\epsilon}\,, \quad E(p) \equiv p^2/2m\,.$$

The $i\epsilon$, $\epsilon \to 0_+$, addition identifies the distribution as a boundary value of an analytic function and indicates how to avoid the pole at a $p_j^2 = p''^2$.

The final result is then

$$\langle \tilde{p}''| \, S^{(\ell)} \, |\tilde{p}'\rangle = -2i\pi\delta(E'' - E') \int \tilde{V}(p'' - p_\ell) \prod_j \frac{\mathrm{d}^d p_j}{(2\pi)^d} \frac{\tilde{V}(p_j - p_{j-1})}{E'' + i\epsilon - E(p_j)} .$$

In this form the perturbation series is a geometric series whose sum satisfies an integral equation, called Lippman–Schwinger's equation. In terms of the operator $T(E)$, where E is generically complex, solution of

$$T(E) = V - VG_0(E)T(E)\,, \quad \text{with} \quad G_0(E) = (H_0 - E)^{-1},$$

the quantity $T(p'', p')$ which appears in equation (3.52) is given by

$$T(p'', p') = \langle p''| \, T(E + i\epsilon) \, |p'\rangle \;\text{ for } E = p'^2/2m = p''^2/2m \,.$$

Exercises

Exercise 3.1

Locality. One considers the operator $U(t)$ defined by its matrix elements:

$$\langle q| U(t) |q'\rangle = \frac{t/\pi}{t^2 + (q-q')^2}.$$

Verify the semi-group property $U(t_1)U(t_2) = U(t_1 + t_2)$.

Show that the corresponding Hamiltonian (as defined by equation (3.6) with $\hbar = 1$) is non-local, that is has a support for $q \neq q'$.

Solution. The matrix elements of the Hamiltonian are

$$\langle q| H |q'\rangle = -\frac{1}{\pi(q-q')^2}\,, \text{ for } q \neq q'\,.$$

Exercise 3.2

The square-well potential. Use the expression obtained for the statistical operator $e^{-\beta H}$ of the harmonic oscillator to derive the spectrum of the attractive square-well potential $H = p^2/2 + \mathcal{V}(x)$ with

$$\mathcal{V}(x) = 0\,, \text{ for } |x| > a/2\,, \quad \mathcal{V}(x) = V < 0\,, \text{ for } |x| < a/2\,.$$

(Exercise requiring some ingenuity).

Solution. The basic idea is to calculate the Fredholm determinant $D(V, E)$ of the operator $H - E$, whose zeros determine the spectrum. The determinant can be expressed in terms of a Gaussian path integral:

$$D^{-1/2}(V, E) \propto \int [\mathrm{d}q(x)] \exp[-\mathcal{S}(q)],$$

$$\mathcal{S}(q) = \int \mathrm{d}x \left[\tfrac{1}{2}\bigl(q'(x)\bigr)^2 + \bigl(\mathcal{V}(x) - E\bigr)q^2(x)\right].$$

This Gaussian integral can be calculated explicitly in various ways. One method is as follows. First, it is convenient to consider the integral as a limit for $\beta \to \infty$ of the partition function in Euclidean time β (that is at temperature $1/\beta$), which is obtained by imposing periodic boundary conditions $q(-\beta/2) = q(\beta/2)$:

$$D^{-1/2}(V, E) \propto \lim_{\beta\to\infty} \operatorname{tr} U(\beta)$$

with

$$\langle q'' |\, U(\beta)\, | q' \rangle = \int_{q(-\beta/2)=q'}^{q(\beta/2)=q''} [\mathrm{d}q(x)] \exp\left[-\mathcal{S}(q)\right].$$

We then split the interval $[-\beta/2, \beta/2]$ into three sub-intervals in which the potential is constant: $[-\beta/2, -a/2]$, $[-a/2, a/2]$, $[a/2, \beta/2]$. We write $U(\beta)$ as a product of statistical operators corresponding to these various intervals. In each interval, the path integral corresponds to the statistical operator of a harmonic oscillator. For what follows, we introduce the notation

$$-E = \tfrac{1}{2}\omega_1^2\,, \ V - E = \tfrac{1}{2}\omega_2^2\,.$$

We denote by U_1 and U_2 the operators corresponding to ω_1 and ω_2, respectively. Then,

$$\operatorname{tr} U(\beta) = \operatorname{tr} U_1(\beta/2 - a/2) U_2(a) U_1(\beta/2 - a/2) = \operatorname{tr} U_1(\beta - a) U_2(a),$$

where the cyclic property of the trace has been used. In the limit $\beta \to \infty$, the operator U_1 becomes the projector on to the ground state of the corresponding oscillator:

$$\operatorname{tr} U(\beta) \underset{\beta\to\infty}{\sim} \sqrt{\frac{\omega_1}{\pi}}\, \mathrm{e}^{-\omega_1(\beta-a)/2} \int \mathrm{d}q'\mathrm{d}q''\ \mathrm{e}^{-\omega_1 q'^2/2}\, \mathrm{e}^{-\omega_1 q''^2/2} \left\langle q'' \right| U_2(a) \left| q' \right\rangle .$$

One then uses the explicit result (3.22) and performs the two Gaussian integrations over q' and q''. One finds

$$\operatorname{tr} U(\beta) \underset{\beta\to\infty}{\sim} \left(\frac{2\omega_1\omega_2}{\sinh(a\omega_2)}\right)^{1/2} \left(\omega_1^2 + \omega_2^2 + 2\omega_1\omega_2 \coth(a\omega_2)\right)^{-1/2} \mathrm{e}^{-\omega_1(\beta-a)/2} .$$

To obtain a result that has a finite limit, it is necessary to normalize the determinant. Dividing it by its value for vanishing potential, one finds

$$\mathrm{e}^{a\omega_1}\, D(V,E)/D(0,E) = \cosh(a\omega_2) + \frac{\omega_1^2+\omega_2^2}{2\omega_1\omega_2}\sinh(a\omega_2).$$

We have calculated for $V-E>0$. The determinant can only vanish for $E>V$. We thus set $\omega_2 = i\kappa_2$. The equation that gives the energies of the bound states can then be written as

$$\tan(a\kappa_2) = \frac{2\omega_1\kappa_2}{\omega_1^2-\kappa_2^2}\,,$$

an equation that can easily be verified by solving the Schrödinger equation for the square-well directly and by combining the two spectral equations that correspond to even and odd eigenfunctions.