4
Semiclassical Expansion; WKB

4.1 Introduction

Classical mechanics is a natural limit of quantum mechanics, therefore the expansion of the action functional S around its value at (or near) a classical system leads to interesting results† in quantum physics.

The expansion, written as follows

$$S(x) = S(q) + S'(q)\cdot\xi + \frac{1}{2!}\,S''(q)\cdot\xi\xi + \frac{1}{3!}\,S'''(q)\cdot\xi\xi\xi + \cdots, \quad (4.1)$$

is constructed in Appendix D.

The role of classical solutions in quantum physics is comparable to the role of equilibrium points in classical dynamical systems, where the time evolution of the system is governed the by dynamical equation

$$dX(t) = f(X(t))dt, \quad (4.2)$$

and an equilibrium point $\bar{x}$ satisfies $f(\bar{x}) = 0$. The nature of the equilibrium point is found from the long time behavior of the nearby motions $x(t)$, which in turn is determined, to a large extent, by the derivative $f'(\bar{x})$ evaluated at the equilibrium point. For example, if the dynamical equation (4.2) reads

$$\left\{\begin{array}{lcl} \frac{dq(t)}{dt} & = & v(t) \\ \frac{dv(t)}{dt} & = & -\mathrm{grad}\left(V(q(t))\right), \end{array}\right. \quad (4.3)$$

† The semiclassical expansion in path integrals has been introduced[**?**] in 1951 for defining the absolute value of the normalization left undefined by Feynman, and for computing approximate values of path integrals. By now there is a very rich literature on semiclassical expansion. For details and proofs of several results presented in this section see reference [18].

then the equilibrium point $(\bar{q}, \bar{v})$ is a critical point, $\mathrm{grad}V(\bar{q}) = 0$, of the potential $V(q)$; its nature is determined by the hessian of V at $\bar{q}$, namely

$$-\frac{\partial^2 V(q)}{\partial \overline{q}^\alpha \partial \overline{q}^\beta}. \tag{4.4}$$

Given an action functional S on a space $\boldsymbol{X}$ of function x, its critical point q, $S'(q) = 0$, is a classical solution; its hessian at q is

$$\mathrm{Hess}(q; \xi, \eta) := S''(q) \cdot \xi\eta.$$

The hessian of the action functional determines the nature of the semiclassical expansion of functional integrals, such as

$$I = \int_{\mathbb{X}} Dx \ \exp\left(\frac{2\pi\imath}{\hbar} S(x)\right) \cdot \phi(x(t_a)). \tag{4.5}$$

Remark The hessian also provides a quadratic form for expressing an action functional integral as a gaussian integral over the variable $\xi \in T_q\boldsymbol{X}$.

The arena for semiclassical expansion consists of the intersection of two spaces: the space U of classical solutions of the action functional S of the system and the domain of integration $\mathcal{P}_{\mu,\nu}M\!\!I^D$ of the functional integral:

Consider a space $\mathcal{P}M\!\!I^D$ of paths $x : \mathbb{T} \to M\!\!I^D$ on a D-dimensional manifold $M\!\!I^D$ (or simply $M\!\!I$); The action functional S is a function

$$S : \mathcal{P}M\!\!I^D \to I\!R, \tag{4.6}$$

defined by a Lagrangian L

$$S(x) = \int_{\boldsymbol{T}} dt \ L(x(t), \dot{x}(t), t). \tag{4.7}$$

Two subspaces of $\mathcal{P}M\!\!I^D$ dominate the semiclassical expansion:

- $U \subset \mathcal{P}M\!\!I^D$, the space of critical points of S

  $$q \in U \ \Leftrightarrow \ S'(q) = 0$$

  i.e. q is a solution of the Euler-Lagrange equations; it follows that U is $2D$ dimensional.
- $\mathcal{P}_{\mu,\nu}M\!\!I^D \subset \mathcal{P}M\!\!I^D$, the space of paths satisfying D initial conditions (μ) and D final conditions (ν).

- Let $U_{\mu,\nu}$ be their intersection,

$$U_{\mu,\nu} := U \cap \mathcal{P}_{\mu,\nu}M\!\!I^D.$$

In section (4.2) the intersection $U_{\mu,\nu}$ consists of only one point q, or several isolated points $\{q_i\}$. In section (**??**) the intersection $U_{\mu,\nu}$ is of dimension $\ell > 0$. In section (4.4) the intersection $U_{\mu,\nu}$ is a multiple root of $S'(q) \cdot \xi = 0$. In section (**??**) the intersection $U_{\mu,\nu}$ is an empty set.

Fig. 4.1. $U_{\mu,\nu} : U \ \cap \ \mathcal{P}_{\mu,\nu}M\!\!I^D$

One can approach $U_{\mu,\nu}$ either from the tangent space T_qU^{2D} to the space U of classical solutions of S, or from the tangent space $T_q\mathcal{P}_{\mu,\nu}M\!\!I^D$ to the domain of integration $\mathcal{P}_{\mu,\nu}M\!\!I^D$

One can also introduce a variation $S + \delta S$ of the action S and approach $U^{2D}(S)$ from $U^{2D}(S + \delta S)$.

4.2 The WKB Approximation

Let the intersection $U_{\mu,\nu}$ of the space U of classical solutions q and the space $\mathcal{P}_{\mu,\nu}M\!\!I^D$ of paths x on $M\!\!I^D$ satisfying D initial conditions (μ) and D final conditions (ν) consist of one simple root q of the Euler-Lagrange equation. The case of $U_{\mu,\nu}$ consisting of multiple *isolated* points $\{q_i\}$ (e.g. the anharmonic oscillator) is similar. Expand the action functional around its value at q

$$S(x) = S(q) + \frac{1}{2}S''(q) \cdot \xi\xi + \Sigma(q;\xi) \quad \text{for} \quad \xi \in T_q\mathcal{P}_{\mu,\nu}M\!\!I^D. \tag{4.8}$$

The WKB approximation consists in dropping $\Sigma(q;x)$ and integrating over the space $T_q\mathcal{P}_{\mu,\nu}M\!\!I^D$ of vector fields ξ

$$I_{\text{WKB}} := \int_{\mathbb{X}_b} D\xi \ \exp\left(\frac{2\pi\imath}{h}\left(S(q) + \frac{1}{2}S''(q) \cdot \xi\xi\right)\right) \cdot \phi(x(t_a)). \tag{4.9}$$

The domain of integration $\boldsymbol{X}_b$ stands for the tangent space $T_q\mathcal{P}_{\mu,\nu}\mathbb{M}^D$ at q of $\mathcal{P}_{\mu,\nu}\mathbb{M}^D$ with D vanishing final conditions (ν)

$$x(t_b) \text{ a fixed point } \Rightarrow \xi(t_b) = 0, \tag{4.10}$$

and D arbitrary initial conditions (ν), to be specified by the choice of the initial "wave function" ϕ. For point-to-point transition, choose,

$$\phi(x(t_a)) = \delta\left(x(t_a) - a\right). \tag{4.11}$$

For momentum-to-point transitions, if $\mathbb{M}^D \neq \mathbb{R}^D$ choose

$$\phi(x(t_a)) = \exp\left(-\frac{1}{s\hbar}\mathcal{S}_0(x(t_a))\right) \cdot \mathcal{T}(x(t_a)), \tag{4.12}$$

where $\mathcal{T}$ is a smooth function on $\mathbb{M}^D$ of compact support and $\mathcal{S}_0$ is an arbitrary, but reasonable, function on $\mathbb{M}^D$. Eq. (4.12) generalizes plane waves on $\mathbb{R}^D$; it is not a momentum eigenstate, but it is adequate† for computing WKB approximations of momentum-to-point transitions.

The space of paths is such that $S''(q) \cdot \xi\xi < \infty$ i.e. an $L^{2,1}$ space (square integrable first derivatives) and $D\xi$ is the canonical Gaussian on $L^{2,1}$ defined by the norm on $L^{2,1}$ [see section 3.2**??**]

$$||\xi||_{L^{2,1}} = \int_{\boldsymbol{T}} dt\ g_{ij}\ \dot{\xi}^i(t)\ \dot{\xi}^j(t). \tag{4.13}$$

When is it justified to replace an integral (4.5) over x by the integral (4.9) over ξ?
If $x(t) \in \mathbb{R}^D$, then in $\mathcal{P}_{\mu,\nu}\mathbb{R}^D$ we can write

$$x = q + \xi$$

$$Dx = D\xi$$

if

$$Q(x) = \frac{1}{2}\int dt\ \left(\dot{x}(t)\right)^2,$$

then

$$Q(q+\xi) = \frac{1}{2}\int dt\ \left(\dot{q}(t)\right)^2 + \int dt\ \dot{q}(t)\ \dot{\xi}(t) + \frac{1}{2}\int dt\ \left(\dot{\xi}(t)\right)^2. \tag{4.14}$$

The first term contributes to $S(q)$, the second contributes to $S'(q)\cdot\xi = 0$,

† See justification in reference 19.

the third term is equal to $Q(\xi)$, and there is no problem in replacing the integral over x by an integral over ξ. The WKB approximation is strictly equivalent to dropping $\Sigma(q;x)$ in the expansion of the action functional S. The neglected contributions can easily be computed.

When $\mathbb{M}^D \neq \mathbb{R}^D$, the contractibility of $\boldsymbol{X}_0$ allows one to map it on to the tangent space of $\mathcal{P}_{\mu,\nu}\mathbb{M}^D$ at q. This technique plays a major role in chapter 7**??** and will be developed there *ab initio*. At this point, we simply compute I_{WKB} given by (4.9) for ϕ a plane wave momentum p_a smoothly limited to a neighborhood of $x(t_a)$

$$\phi(x(t_a)) = \exp\left(-\frac{1}{s\hbar}\,\langle p_a, x(t_a)\rangle\right)\mathcal{T}(x(t_a)). \tag{4.15}$$

Momentum-to-position transitions

The WKB approximation (4.9) is then given explicitly by

$$\begin{aligned} I_{\mathrm{WKB}}(b,t_b;p_a,t_a) &= \exp\frac{2\pi\imath}{h}\mathcal{S}\left(x_{\mathrm{cl}}(t_b),p_{\mathrm{cl}}(t_a)\right) \\ &\quad\times\left(\det\frac{\partial^2\mathcal{S}}{\partial x^i_{\mathrm{cl}}(t_b)\partial p_{\mathrm{cl}\ j}(t_a)}\right)^{1/2}. \end{aligned} \tag{4.16}$$

We outline a proof of this well-known formula. The terms independent of ξ, namely

$$S(q) + \langle p_a, x(t_a)\rangle = \mathcal{S}(x_{\mathrm{cl}}(t_b),p_{\mathrm{cl}}(t_a)) \tag{4.17}$$

combine to give the action function. The integral over ξ yields the determinant of the hessian of the action function. First we compute

$$\int_{\mathbb{X}}\mathcal{D}_{Q_0}\xi\ \exp\frac{\pi\imath}{h}(Q_0(\xi)+Q(\xi)) \tag{4.18}$$

where $Q_0(\xi)+Q(\xi) = S''(q)\xi\xi$ and $Q_0(\xi)$ is the kinetic energy contribution to the second variation. Integrals similar to (4.18) occur frequently, and we shall set (4.18) in a slightly more useful form. We shall again use the properties of linear mappings. So far we have exploited the formula

$$\int_{\mathbb{X}} D\gamma_{\mathbb{X}}\ (f\circ L)(x) = \int_{\boldsymbol{Y}} D\gamma_{\boldsymbol{Y}}(y)\ f(y), \tag{4.19}$$

where $L : \boldsymbol{X} \to \boldsymbol{Y}$ linearly and the Gaussian integrators are defined by the quadratic form $W_{\mathbb{X}}$ and $W_{\boldsymbol{Y}}$ such that

$$W_{\boldsymbol{Y}} = W_{\mathbb{X}}\circ\tilde{L} \tag{4.20}$$

Now we consider the inverse process†.

Given two quadratic forms, say $Q_{\mathbb{X}}$ and $Q_{\boldsymbol{Y}}$, find the linear map which maps the Gaussian $D\gamma_{\mathbb{X}}$ into $D\gamma_{\boldsymbol{Y}}$.

Fig. 4.2. linear maps

The key equation is now

$$Q_{\mathbb{X}} = Q_{\boldsymbol{Y}} \circ L. \tag{4.21}$$

We do not introduce L^{-1} because the results are valid when L is not invertible. In order to display Q explicitly we use the qualified equality‡

$$D\gamma_{\mathbb{X}}(x) \stackrel{\int}{=} D_{\mathbb{X}}(x)\ \exp\Big(-\frac{\pi}{s} Q_{\mathbb{X}}(x)\Big), \tag{4.22}$$

where $D_{\mathbb{X}}(x)$ is a dimensionless volume element.

In finite dimensions

$$\begin{aligned} Q(x) &= Q_{ij}\ x^i x^j, \\ Dx &= dx^1 \cdots dx^D\ |\det Q_{ij}|^{1/2}, \\ (Lx)^i &= L^i{}_j x^j =: y^i, \\ D(Lx) &= \det L \cdot Dx. \end{aligned} \tag{4.23}$$

† Exploiting the inverse process for solving several different problems can be found in ref[20][**?**]. For oscillatory integral (s=i), and for precise mathematical proof see ref[19][**?**].

‡ Equality of terms defined by the same integral.

It follows from (4.20) that

$$(Q_{\mathbb{X}})_{ij} = (Q_{\boldsymbol{Y}})_{k\ell}\ L^k{}_i L^\ell{}_j; \tag{4.24}$$

hence

$$\det Q_{\mathbb{X}} = \det Q_{\boldsymbol{Y}}\,(\det L)^2\,. \tag{4.25}$$

In order to complete rapidly the calculation of (4.9) we assume that the simple dimensionless equations (4.23) and (4.25) are valid in the infinite dimensional case. Infinite dimensional determinants are discussed in section 10.3**??**.

Proposition If $s = 1$, i.e. if $Q_{\mathbb{X}}$ and $Q_{\boldsymbol{Y}}$ are positive definite, then

$$\int_{\mathbb{X}} D_{\boldsymbol{Y}}x\ \exp(-\pi Q_{\mathbb{X}}(x)) = \det\left(Q_{\mathbb{X}}/Q_{\boldsymbol{Y}}\right)^{-1/2}. \tag{4.26}$$

If $s = \imath$, i.e. for oscillatory integrals, then

$$\int_{\mathbb{X}} D_{\boldsymbol{Y}}x\ \exp(\imath\pi Q_{\mathbb{X}}(x)) = \left|\det\left(Q_{\mathbb{X}}/Q_{\boldsymbol{Y}}\right)\right|^{-1/2} \imath^{\mathrm{Ind}(Q_{\mathbb{X}}/Q_{\mathbb{Y}})} \tag{4.27}$$

where the index† $\mathrm{Ind}(Q_{\mathbb{X}}/Q_{\boldsymbol{Y}})$ counts the number of negative eigenvalues of $Q_{\boldsymbol{Y}}$ w.r.t. $Q_{\mathbb{X}}$.

Proof

$$\begin{aligned}
d\gamma_{\boldsymbol{Y}}(Lx) &= D_{\boldsymbol{Y}}(Lx)\ \exp\Big(-\frac{\pi}{s}Q_{\boldsymbol{Y}}(Lx)\Big)\,,\\
d\gamma_{\boldsymbol{Y}}(Lx) &= |\det L|\, D_{\boldsymbol{Y}}x\ \exp\Big(-\frac{\pi}{s}(Q_{\boldsymbol{Y}}\circ L)\Big)\,(x), &(4.28)\\
d\gamma_{\boldsymbol{Y}}(Lx) &= \left|\det Q_{\mathbb{X}}/\det Q_{\boldsymbol{Y}}\right|^{1/2}\ D_{\boldsymbol{Y}}x\ \exp\Big(-\frac{\pi}{s}Q_{\mathbb{X}}(x)\Big)\,. &(4.29)
\end{aligned}$$

Integrating both sides gives the proposition (4.25). In the case $s = \imath$ (i.e. eq. (4.26)), the phase reflects the fact that

$$\int_R \frac{du}{\sqrt{|a|}}\ \exp\Big(\pm\imath\pi\frac{u^2}{|a|}\Big) = \exp\Big(\pm\frac{\imath\pi}{4}\Big)\,. \tag{4.30}$$

□

† See for instance reference [19][**?**], p. 2287, p. 2301, and reference [20][**?**] pp. 318-319 for comments and references on the phase of the propagator (4.27).

Remarks

(i) Equation (4.26) is a version of the Cameron-Martin formula, simplified by using (4.22) which breaks the Gaussian volume element into a translation invariant term and the exponential of a quadratic term.

(ii) Equation (4.26-4.27) rests on the linear map $L : \boldsymbol{X} \to \boldsymbol{Y}$, but can be used without identifying L.

The determinants in (4.26) (4.27) are infinite dimensional. It remains to prove that their ratio is a finite Van Vleck–Morette determinant — the finite determinant in (4.16) for momentum to position transitions, or the finite determinant (4.30) for point to point transitions. There are many lengthy proofs of this remarkably useful fact. Each author favors the proof using his/her previously established results. We shall give the gist of side proofs with references and apologies for not quoting all the proofs and following Kac's advice [**?**] "one should try to formulate even familiar things in as many different ways as possible"!

Finite dimensional determinants

(i) In the discretized version of path integrals[**?**][**?**] the infinite limit of the product of the short time normalizations is shown to be the square root of a jacobian which appears if one changes the past description from momenta (at discretized times) to points (at discretized times). In modern parlance, this says that the point-to-point determinant (4.25) can be obtained from a phase space path integral[**?**] which has a short time propagator normalized to unity.

(ii) The prodistribution definition of path integrals[23][**?**][31][**?**][38][**?**][eq. B.18] generalizes the definition of oscillatory integrals over $\mathbb{R}^n$ to integrals over spaces which are not necessarily locally compact. Prodistribution can be used on topological vector spaces $\boldsymbol{X}$ that are Hausdorff and locally convex. In brief one works with the projective system of $\boldsymbol{X}$ — that is a family of finite dimensional quotient space of $\boldsymbol{X}$ indexed by closed subspaces of finite codimension. The word "prodistribution" stands for "projective family of distributions", like "promeasure" stands for "projective family of measures". In spite of their sophisticated names, prodistrbutions are a very practical tool — to quote only one application, they are

usefull in obtaining as closed form glory scattering cross-section [12][**?**].

Showing that the infinite dimensional determinants (4.26, 4.27) on $\boldsymbol{X}$ are equal to finite Van Vleck-Morette determinants can be done as follows. Choose the projective system on $\boldsymbol{X}$ indexed by closed subspaces V, W, etc. where

$$V \text{ is the set of functions } f \text{ vanishing on a partition } \theta_v = \{t_1, \ldots, t_v\}. \tag{4.31}$$

The quotient $\boldsymbol{X}/V$ is the v-dimensional space of functions f defined by $\{f(t_1), \ldots, f(t_v)\}$.

The reader may wonder if it is worthwhile to introduce projective systems when they lead to spaces such as $\boldsymbol{X}/V$ which discretization introduces right away. The answer is that discretization deals with meaningless limits of integrals over $I\!R^n$ when n tends to infinity, whereas projective systems deal with families of meaningful projections of $\boldsymbol{X}$ on $I\!R^v$, $I\!R^w$, etc.... There are many choices of projective systems of a space $\boldsymbol{X}$. We choose one which shows how prodistributions relate to discretization; it is also a practical choice for the computation of ratio of infinite dimensional determinants. The work is a certain amount of algebra on finite dimensional spaces.

(iii) A generalized Cameron-Martin formula [**?**][**?**]†
Determinants are objects defined by linear mappings; therefore the Cameron-Martin formula which deals with gaussian integrals under a linear change of variable of interaction, provides a tool for computing (4.25). Let (see fig 4.1)

$$\begin{array}{rcl} L : \boldsymbol{X} \to \boldsymbol{Y} & \text{by} \ \ \xi \mapsto \eta & \text{such that} \quad Q_{\boldsymbol{X}} = Q_{\boldsymbol{Y}} \circ L \\ \tilde{L} : \boldsymbol{Y}' \to \boldsymbol{X}' & \text{by} \ \ \eta' \mapsto \xi' & \text{such that} \quad W_{\boldsymbol{Y}'} = W_{\boldsymbol{X}'} \circ \tilde{L} \end{array} \tag{4.32}$$

$$W_{\boldsymbol{X}'}(x') = \langle x', G_{\boldsymbol{X}'} x' \rangle \ \text{ and similarly for } W_{\boldsymbol{Y}'}.$$

$$\det(Q_{\boldsymbol{X}}/Q_{\boldsymbol{Y}})^{1/2} = \det L = \det \tilde{L} = \det(G_{\boldsymbol{Y}'}/G_{\boldsymbol{X}'})^{1/2} \tag{4.33}$$

For a momentum-to-point transition (Appendix IE, E.24)

$$G_{\boldsymbol{X}}(r,s) \quad = \quad \theta(s-r) K(r,t_a) N(t_a,t_b) J(t_b,s)$$

† These are generalizations and several versions of the original Cameron-Martin formula useful in a variety of applications. A number of them can be found in the above references.

$$-\theta(r-s)J(r,t_b)\tilde{N}(t_b,t_a)\tilde{K}(t_a,s). \quad (4.34)$$

In (4.25) the quadratic form $Q_{\boldsymbol{Y}}$ is the kinetic energy. For paths $\xi : \mathbb{T} \to \mathbb{R}$ and $m = 1$, $Q_{\boldsymbol{Y}}(\xi) = \frac{1}{2}\int_{\boldsymbol{T}} dt\dot{x}^2(t)$;

$$G_{\boldsymbol{Y}}(r,s) = \theta(s-r)(t_b-s) - \theta(r-s)(r-t_b). \quad (4.35)$$

The linear map $\tilde{L} : \boldsymbol{Y}' \to \boldsymbol{X}'$ by $\eta' \mapsto \xi'$ is explicitly given by

$$\xi'(t) = \eta'(t) + \int_{\boldsymbol{T}} dr\theta(r-t)\frac{dK}{dr}(r,t_a)N(t_a,r)\eta'(r). \quad (4.36)$$

With an explicit expression for $\tilde{L}$, we use the fundamental relation between determinant and trace

$$d\log\det\tilde{L} = \mathrm{Tr}\tilde{L}^{-1}d\tilde{L}. \quad (4.37)$$

After some calculations†

$$\begin{aligned}\det\tilde{L} &= (\det K(t_b,t_a)/\det K(t_a,t_a))^{1/2} \quad (4.38)\\ &= (\det K(t_b,t_a))^{1/2}.\end{aligned}$$

The inverse of the Jacobi matrix K is the hessian of the classical action function $\mathcal{S}(x_{\mathrm{cl}}(t_b), p_{\mathrm{cl}}(t_a))$

$$\det\tilde{L} = \left(\det\frac{\partial^2\mathcal{S}}{\partial x^i_{\mathrm{cl}}(t_b)\ \partial p_{\mathrm{cl}\,j}(t_a)}\right)^{-1/2}. \quad (4.39)$$

Equation (4.16) follows. □

(iv) Varying the integration [78[**?**] JMP 1995]
Eq. (4.16) is fully worked out in [78[**?**] pp. 2254-2259]. The strategy for computing $\det(Q_{\mathbb{X}}/Q_{\boldsymbol{Y}})$ where

$$Q_{\boldsymbol{Y}}(\xi) = Q_0(\xi), Q_{\mathbb{X}}(\xi) = Q_0(\xi) + Q(\xi) = S''(q)\xi\xi$$

consists introducing a one parameter action functional $S_\nu(x)$ such that

$$S''_\nu(q)\xi\xi = Q_0(\xi) + \nu Q(\xi) =: Q_\nu(\xi). \quad (4.40)$$

Physical arguments as well as previous calculations suggest that $\det(Q_0/Q_1)$ is equal to $\det K^i_j(t_b,t_a)$ where the Jacobi matrix K is defined (Appendix IE) by

$$K^i_j(t_b,t_a) = \partial x^i_{\mathrm{cl}}(t_b)/\partial x^j_{\mathrm{cl}}(t_a). \quad (4.41)$$

† The calculations are explicitly given in [38[**?**] and 27[**?**]]; they can be simplified by using the qualified equality (4.21).

From the one-parameter family of action functionals $S_\nu(x) \equiv S(\nu; x)$ one gets a one parameter family of Jacobi matrices.

$$K^i_j(\nu; t_b, t_a) = \partial x^i_{\rm cl}(\nu; t_b)/\partial x^j_{\rm cl}(\nu; t_a) \tag{4.42}$$

Set

$$c(\nu) := \det K(\nu; t_b, t_a)/K(0; t_b, t_a). \tag{4.43}$$

A nontrivial calculation [78[**?**]] proves that $c(\nu)$ satisfies the same differential equation and the same boundary condition as $\det(Q_0/Q_\nu)$.

(v) Varying the end points of a classical path [Appendix IE eqs. (E.33) to (E.44)]
This method gives the Van Vleck-Morette determinant for the position-to-position transitions (4.45). Let $u = (x_a, x_b)$ characterize the end points of the classical path $x_{\rm cl}(u)$. To the action functional $S(x_{\rm cl}(u))$ corresponds an action function $\mathcal{S}$:

$$S(x_{\rm cl}(u)) = \mathcal{S}(x_{\rm cl}(t_a; u), x_{\rm cl}(t_b; u)). \tag{4.44}$$

By taking the derivatives with respect to x_a and x_b (i.e. w.r.t. the D-components of x_a and the D-components of x_b) of both sides of (4.44), one obtains an equality between the ratio of two infinite dimensional determinants (l.h.s.) and a finite dimensional determinant (r.h.s.). The calculation is spelled out in Appendix IE.

(vi) Varying the action functional [Bryce[**?**]]
The method is worked out explicity for the cas of position-to-position transitions in (4.45) [Bryce[**?**] pp. 339-341]. The variation of the action functional induces a variation of its hessian more general than the variation of the hessian in (4.40). Consider two green functions of the same Jacobi operator, but with different boundary conditions such that their difference is expressed in terms of a Jacobi matrix. The variation of the ratio of the determinants of these green's functions can be expressed in terms of the trace of their differences (4.37), i.e. in terms of the trace of a Jacobi matrix. Using again the trace determinant eq. (4.37), one arrives at an equation between the ratio of infinite dimensional determinants and a finite dimensional determinant.

Point-to-point transitions

A derivation similar to the derivation of (4.16) yields

$$I_{\rm WKB}(b,t_b;x_a,t_a) = \exp\frac{2\pi\imath}{h}\mathcal{S}(x_{\rm cl}(t_b),x_{\rm cl}(t_a))\cdot\left(\det\frac{\partial^2\mathcal{S}}{\partial x^i_{\rm cl}(t_b)\,\partial x^j_{\rm cl}(t_a)}\right)^{1/2} \tag{4.45}$$

where $\mathcal{S}$ is the classical function evaluated for the classical path defined by $x_{\rm cl}(t_b) = b$, $x_{\rm cl}(t_a) = a$.

4.3 An example: The anharmonic oscillator

The one-dimensional quartic anharmonic oscillator is a particle of mass m in a potential

$$V(x) = \frac{1}{2}m\omega^2x^2 + \frac{1}{4}\lambda x^4. \tag{4.46}$$

Maurice Mizrahi [15[**?**]] used path integrals, as developed here†, for computing the semiclassical expansion of the anharmonic oscillator propagator.

$$\langle x_b,t_b|x_a,t_a\rangle = \int_{\mathbb{X}_{a,b}}\mathcal{D}x\,\exp\left(2\pi\imath\frac{1}{h}\int_{\boldsymbol{T}}dt\left(\frac{m}{2}\dot{x}^2(t) - V(x(t))\right)\right). \tag{4.47}$$

In this section we present only the highlights of Mizrahi's work; we refer to his publications [15[**?**]] for proofs and explicit formulae.

The Potential

The shape of the potential changes drastically as λ changes sign, and the semiclassical expansion is not analytic in λ. In some neighborhood of the origin, $x = 0$, there exists a potential well and a harmonic motion for $\lambda > 0$ and $\lambda < 0$; for $\lambda > 0$ there is a stable ground state, but for

† In early works eq. (2.25**??**) reads

$$\int d\omega(x) = \exp(-\imath\,\langle x',x\rangle) = \exp(\imath W(x')),$$

where $d\omega(x)$ has not been decomposed into a translation invariant term $\mathcal{D}_Q x$ and the exponential of a quadratic term $Q(x)$, "inverse" of $W(x')$. The "inverse" of $W(x')$ was labeled $W^{-1}(x)$.

$\lambda < 0$ the ground state is unstable. For large x, the x^4-term dominates the x^2-term, regardless of the magnitude of λ. Consequently perturbation expansions in powers of λ are doomed to failure. Non-analyticity at $\lambda = 0$ does not mean singularity at $\lambda = 0$.

Perturbation expansions in powers of the coupling constant λ have led to the conclusion that there is a singularity at $\lambda = 0$, but the conclusion of Mizrahi's non perturbative calculation reads as follows:

"The folkloric singularity at $\lambda = 0$ does not appear at any stage, whether in the classical paths, the classical action, the Van Vleck-Morette function, the Jacobi fields, or the Green's functions, in spite of report to the contrary."

We present Mizrahi's proof because it is simple and because it clarifies the use of boundary conditions in ordinary differential equations. Recall that boundary conditions are necessary for defining the domain of integration of a path integral.

The classical system

The dynamical equation satisfied by the classical solution q is

$$\ddot{q}(t) + \omega^2 q(t) + \frac{\lambda}{m} q^3(t) = 0. \tag{4.48}$$

If we set $m = 1$ then the mass can be restored by replacing λ by λ/m. The dynamical equation can be solved in terms of biperiodic elliptic functions (See Appendix IF). The solution may be expressed in terms of any elliptic function. For example, assuming $\lambda > 0$, we choose

$$q(t) = q_m \mathrm{cn}(\Omega(t - t_0), k) \tag{4.49}$$

and insert $q(t)$ in (4.48) for determining Ω and k

$$\left\{ \begin{array}{rcl} \Omega^2 & = & \omega^2 + \lambda q_m^2 \\ k^2 & = & \frac{1}{2}\lambda \left(\frac{q_m}{\Omega}\right)^2; \quad \text{note that } 0 \leq 2k^2 \leq 1. \end{array} \right.$$

Therefore,

$$\left\{ \begin{array}{rcl} q_m & = & \left(\frac{2k^2\omega^2}{\lambda(1-2q^2)}\right)^{1/2} \\ q(t) & = & q_m \mathrm{cn}\left(\frac{\omega(t-t_o)}{(1-2k^2)^{1/2}}, k\right) \end{array} \right. \tag{4.50}$$

For arbitrary values of the constants of integration (k^2, t_0) the classical

solution has a $\lambda^{-1/2}$ singularity at $\lambda = 0$. If we instead choose "physical" boundary conditions such as

$$q(t_a) = q_a \quad \text{and} \quad \dot{q}(t_a) = \sqrt{a}$$

$$\begin{cases} q(t) &= A^{1/2}\cos(\omega(t-t_a) - \arccos q_a A^{-1/2}) \\ A &= \left(\frac{\sqrt{a}}{\omega}\right)^2 + q_a^2 \end{cases} \tag{4.51}$$

the classical solution has no singularity at $\lambda = 0$; it approaches harmonic motion as λ tends to 0.

There is a countably infinite number of possible values for k^2.

For the quantum system (4.32) one needs to define the classical paths by endpoint boundary conditions

$$q(t_a) = x_a, \quad q(t_b) = x_b. \tag{4.52}$$

The endpoint boundary conditions (4.37) are satisfied only when k^2/λ is a constant (possibly depending on ω). There is only one solution for k† that satisfies (4.50, 4.52) *and* goes to zero when λ goes to zero. This solution corresponds to the lowest energy system; this is the classical solution we choose for expanding the action functional. This solution is not singular at $\lambda = 0$; indeed it coincides with the (generally) unique harmonic oscillator path between the two fixed endpoints.

Remark: The use of "physical" boundary conditions versus the use of arbitrary boundary conditions, possibly chosen for mathematical simplicity, can be demonstrated on a simpler example: consider the fall of a particle, slowed by friction at a rate proportional to k; the solution of the dynamical equation appears to be singular when $k \longrightarrow 0$ if expressed in terms of arbitrary constants of integration; but it tends to free fall when expressed in terms of physical constants of integration.

The Quantum System

The WKB approximation of a point-to-point transition is given by (4.45). The quantities appearing in (4.45) can all be constructed from the solu-

† The infinite number of classical paths for the harmonic oscillator that exist when $\omega(t_b - t_a) = n\pi$ is a different phenomenon which is analyzed in section (**??**) on Caustics.

tions of the Jacobi operator equation. (See Appendix IE)

$$\left(-\frac{d^2}{dt^2} - \omega^2 - 3\lambda q^2(t)\right) f(t) = 0 \tag{4.53}$$

The action function $\mathcal{S}(x_a, x_b)$ and the determinant of its hessian have been computed explicitly in terms of elliptic functions by Mizrahi[**?**] for the anharmonic oscillator.

The expansion of the action functional (4.1) provides a quadratic form

$$Q(\xi) := S''(q) \cdot \xi\xi \tag{4.54}$$

which is useful for defining a gaussian volume element.

$$\mathcal{D}_Q\xi \, \exp\left(\frac{2\pi\imath}{h} Q(\xi)\right) =: d\gamma_Q(\xi) \tag{4.55}$$

The full propagator (4.32) is given by a sum of gaussian integrals of polynomials in ξ, with the gaussian volume element $d\gamma_Q(\xi)$. The full propagator is an asymptotic expansion

$$K = I_{\mathrm{WKB}}(1 + hK_1 + h^2K_2 + \ldots). \tag{4.56}$$

The term of order n consists of an n-tuple ordinary integral of elliptic functions; see [**?**] for explicit expressions of I_{WKB} and K_1. The expansion is asymptotic because the elliptic functions depend implicitly on λ.

A prototype for the $\lambda\phi^4$ model

To what extent is the anharmonic oscillator a prototype for the $\lambda\phi^4$ model in quantum field theory?

Both systems are nonlinear systems which admit a restricted superposition principle. Indeed, the dynamical equation for the $\lambda\phi^4$ self-interaction, namely $(\Box - m^2)\phi - \lambda\phi^3 = 0$, can be readily reduced to the dynamical equation for the one-dimensional anharmonic oscillator, namely

$$\bar{\phi}'' - m^2\bar{\phi}/K^2 - \lambda\bar{\phi}^3/K^2 = 0 \quad \text{where} \quad \phi(x_1, x_2, x_3, x_4) \equiv \bar{\phi}(K \cdot x), \tag{4.57}$$

where K is an arbitrary 4-vector (plane wave solution). The elliptic functions which are solutions of this equation are periodic, and admit a restricted superposition principle, rare for nonlinear equations: If an elliptic cosine (cn) with a certain modulus k_1 is a solution, and if an

elliptic sine (sn) with another modulus k_2 is also a solution, then the linear combination (cn + ısn) is also a solution[**?**], but the common modulus k_3 is different from k_1 and k_2.

The gaussian technology developed for path integrals can be used to a large extent for functional integrals in Quantum Field Theory. In the case of the anharmonic oscillator, the gaussian volume elements for free particles and for harmonic oscillators lead to a "folkloric" singularity. Mizrahi's work has shown that for coherent results, one must use the gaussian volume element defined by the second variation of the action functional. To the best of our knowledge, such a gaussian volume element has not been used in the $\lambda\phi^4$ model (see footnote in section 16.2).

A major difference between systems in quantum mechanics and quantum field theory comes from the behavior of the two-point functions, which are the preferred covariance for gaussian volume elements. Consider, for example, covariances defined by $-\frac{d^2}{dt^2}$

$$-\frac{d^2}{dt^2}G(t,s) = \delta(t,s) \tag{4.58}$$

and by a laplacian in D-dimension

$$\Delta_x\, G(x,y) = \delta(x,y). \tag{4.59}$$

The covariance $G(t,s)$ is continuous; the covariance $G(x,y)$ is singular at $x = y$. The situation $G(x,y) \simeq |x-y|^{2-D}$ is discussed in section 2.5. Renormalization schemes are needed in Quantum Field Theory and are introduced in chapter 14-15-16.

4.4 Incompatibility with Analytic Continuation

A word of caution for semiclassical physics: The laplacian, or its generalizations, is the highest order derivative term and determines the nature of the equation, but the Laplacian contribution vanishes when $\hbar = 0$. Therefore the solutions of the Schrödinger equation have an essential singularity at the origin of a complexified $\hbar$ plane. Care must be taken when using analytic continuation together with expansions in powers of $\hbar$. Michael Berry[**?**] gives an illuminating example in the study of

scent weakly diffusing in random winds. Berry works out the probability that the pheromones emitted by a female moth reach a male moth given a realistic diffusion constant D. Diffusion alone cannot account for males picking up scents from hundreds of meters away. In fact females emit pheromones only when there is a wind so that diffusion is aided by convection. The concentration of pheromones looks like a Schrödinger equation if one sets $D = i\hbar$. However, the limit as $D \longrightarrow 0$ (convection dominated transport) is utterly different from the limit $\hbar \longrightarrow 0$. This reflects the fact that the solutions of the concentration equation have an essential singularity at the origin of the complexified D-plane, and behave differently if $D = 0$ is approached along the real axis (convection-diffusion) or imaginary axis (quantum mechanics). The creative aspects of singular limits, in particular the quantum-classical limit, are praised by Berry in an article of Physics Today (May 2002), whereas in 1828 Niels Henrik Abel wrote that divergent series "are an invention of the devil."