

The Semi-classical Approximation for Pedestrians an elementary introduction

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Abstract

These lectures are intended to introduce the Semi Classical Approximation and some of its intricacies in a consistent and transparent way. The main topics to be covered are

- The semi classical approximation for the quantum evolution operator.
- Uniform approximations
- Semi-classical spectral theory:
- The trace formula and some of its applications. (For systems in 1-d)

It is hoped that the ideas and tools presented here will provide a solid jumping-board for further studies and applications.

"Putting quantum flesh on classical bones" (W.H. Miller)

Motivation (For Physicists)

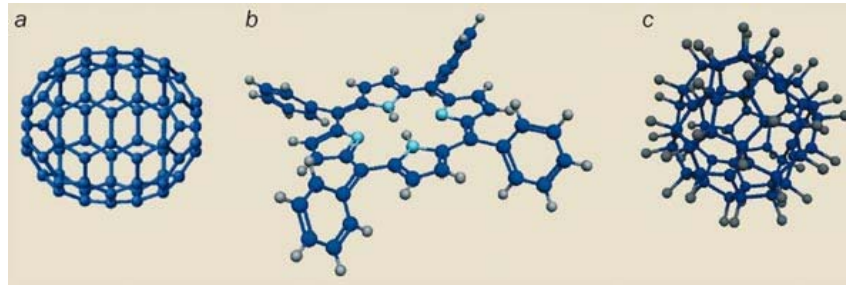
The correspondence principle in action!

A two slits experiment with heavy molecules

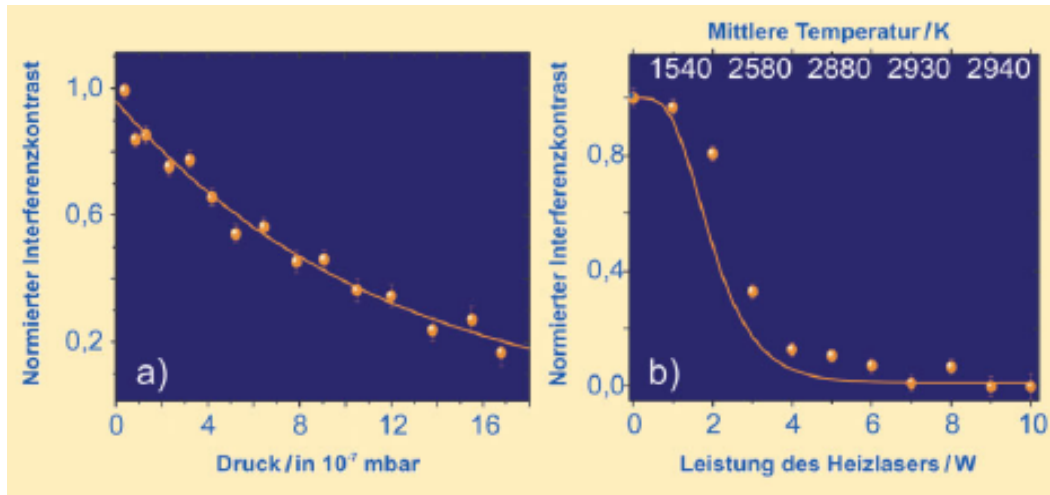
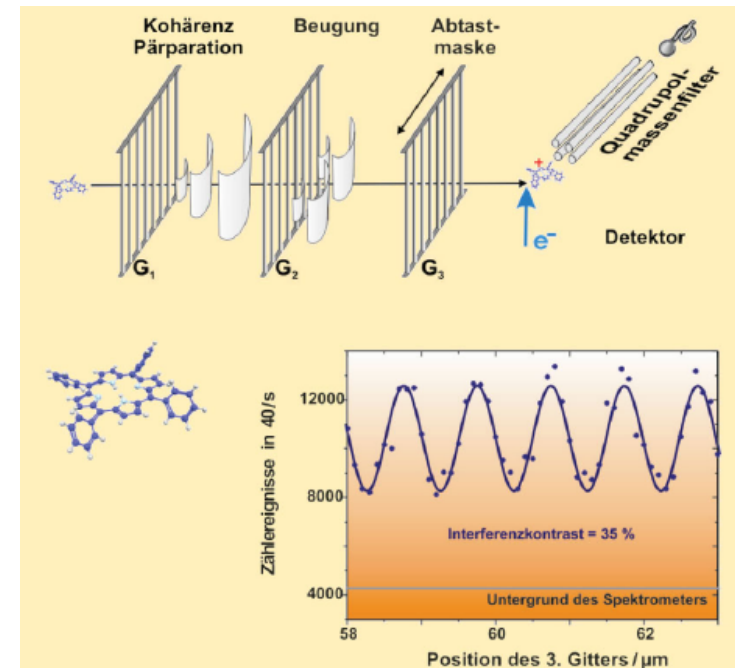
Probing the limits of the quantum world

M. Arndt, K. Hornberger, and A. Zeilinger,

[Physics World \(March 2005\) 35-40](#)



- a) The buckyball carbon-70;
- b) The pancake-shaped biomolecule tetraphenylporphyrin (TPP) $C_{44}H_{30}N_4$;
- c) The fluorinated fullerene $C_{60}F_{48}$. (atomic mass of 1632 units)



Motivation (For Mathematicians)

1. Singular perturbation theory:

The Schroedinger equation:

$$\left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + v(x) \right] \phi(x, t) = i\hbar \frac{\partial}{\partial t} \phi(x, t)$$

$\hbar \rightarrow 0?$

2. Oscillatory integrals

$$\int dx e^{if(x) = \hbar}$$

Bibliography

Books

Richard P. Feynman and Albert R. Hibb:
Quantum Mechanics and Path Integrals
(McGraw-Hill, New York, 1965).

L. S. Schulman:

Techniques and Applications of Path Integration,
(Wiley -Interscience Monographs and Texts in Physics and Astronomy, NY, 1981)

David J. Tannor:

Introduction to Quantum Mechanics –A time dependent perspective.
(University Science Books, 2007)

<http://www.weizmann.ac.il/chemphys/tannor/Book/>

Articles

Too many to be listed.

These lectures are based on my papers with S. Levit, K. Moehring and David Brink.

To download: <http://www.weizmann.ac.il/complex/uzy/publications.html>

26,27,29,30,38,39,41,47

Preliminaries: Classical vs Quantum evolution

★ Classical Evolution:

$$L(\mathbf{q}, \dot{\mathbf{q}}; t) = \frac{m}{2} \dot{\mathbf{q}}^2 - V(\mathbf{q}, t) \quad ; \quad \mathbf{q} \in R^f \quad ; \quad \dot{\mathbf{q}} = \frac{d\mathbf{q}}{dt}$$

$$H(\mathbf{p}, \mathbf{q}, t) = \frac{1}{2m} \mathbf{p}^2 + V(\mathbf{q}, t) \quad ; \quad \mathbf{p} \in R^f$$

★ Quantum Evolution operator (propagator) $K(\mathbf{q}''t''; \mathbf{q}'t')$ $\forall t'' > t'$:

$$\left(-\frac{\hbar^2}{2m} \Delta_{\mathbf{q}''} + V(\mathbf{q}'', t'') \right) K(\mathbf{q}''t''; \mathbf{q}'t') = i\hbar \frac{\partial}{\partial t''} K(\mathbf{q}''t''; \mathbf{q}'t')$$

$$K(\mathbf{q}''t''; \mathbf{q}'t') = 0 \quad \text{for } t'' < t' \quad ; \quad \lim_{t'' \downarrow t'} K(\mathbf{q}''t''; \mathbf{q}'t') = \delta(\mathbf{q}'' - \mathbf{q}')$$

$$\Psi(\mathbf{q}'', t'') = \int d\mathbf{q}' K(\mathbf{q}''t''; \mathbf{q}'t') \Psi(\mathbf{q}', t')$$

The transition-probability density is $P(\mathbf{q}''t''; \mathbf{q}'t') = |K(\mathbf{q}''t''; \mathbf{q}'t')|^2$

Composition (semigroup property) $\forall t'' > t > t'$:

$$K(\mathbf{q}''t''; \mathbf{q}'t') = \int d\mathbf{q} K(\mathbf{q}''t''; \mathbf{q}t) K(\mathbf{q}t; \mathbf{q}'t')$$

Unitarity :

$$\int d\mathbf{q}' K(\mathbf{q}''t''; \mathbf{q}'t') K^*(\mathbf{q}'''t''; \mathbf{q}'t') = \delta(\mathbf{q}''' - \mathbf{q}'')$$

Spectral decomposition for time independent H

$$K(\mathbf{q}''t''; \mathbf{q}'t') = \langle \mathbf{q}'' | e^{-\frac{i}{\hbar}H(t''-t')} | \mathbf{q}' \rangle = \sum_n \psi_n(\mathbf{q}'') \psi_n^*(\mathbf{q}') e^{-\frac{i}{\hbar}E_n(t''-t')}$$

Free propagation:

$$K_{free}(\mathbf{q}''t''; \mathbf{q}'t') = \left(\frac{m}{2\pi i \hbar T} \right)^{\frac{f}{2}} e^{i \frac{m}{2} \frac{|\mathbf{q}'' - \mathbf{q}'|^2}{T}} ; \quad T = t'' - t' .$$

Exercise 1:

- Check by substitution that $K_{free}(\mathbf{q}''t''; \mathbf{q}'t')$ satisfies the time dependent Schrödinger equation for a free particle in f dimensions.
- Prove that $\lim_{t'' \downarrow t'} K_{free}(\mathbf{q}''t''; \mathbf{q}'t') = \delta(\mathbf{q}'' - \mathbf{q}')$.

Feynman Path Integral representation

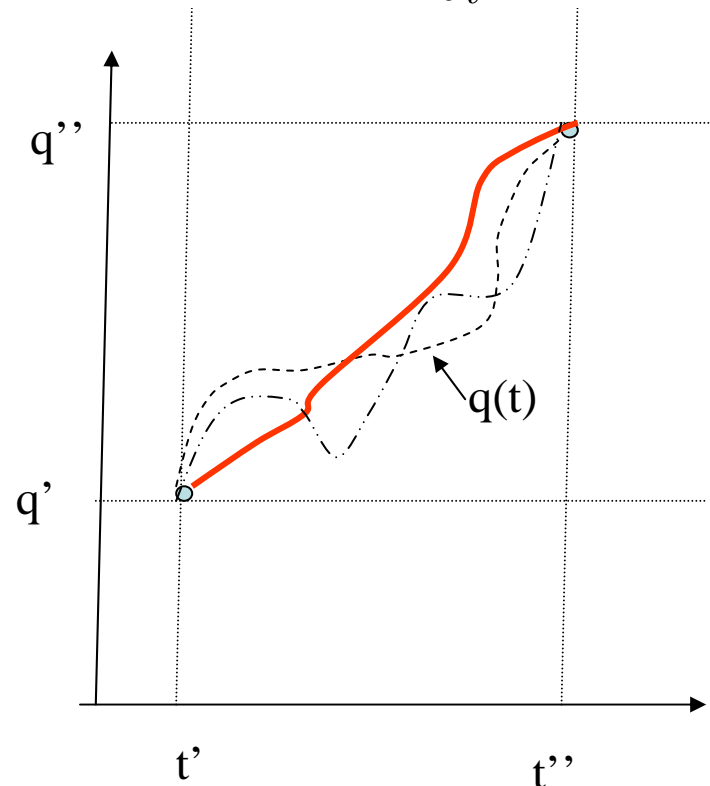
The Democracy of Paths:

Richard P. Feynman and Albert R. Hibbs,
Quantum Mechanics and Path Integrals
(McGraw-Hill, New York, 1965).

$$K(\mathbf{q}''t''; \mathbf{q}'t') = \int D[\mathbf{q}(t)] \exp \left[i \frac{S[\mathbf{q}(t)]}{\hbar} \right].$$

$\mathbf{q}(t)$ a piecewise \mathcal{C}^1 path in config. space from \mathbf{q}' at t' to \mathbf{q}'' at t'' :
 $\mathbf{q}(t') = \mathbf{q}'$ and $\mathbf{q}(t'') = \mathbf{q}''$.

$S[\mathbf{q}(t)]$ the action functional: $S[\mathbf{q}(t)] = \int_{t'}^{t''} dt L(\mathbf{q}(t), \dot{\mathbf{q}}(t); t)$.



To define the integral, Feynman proposes the limit:

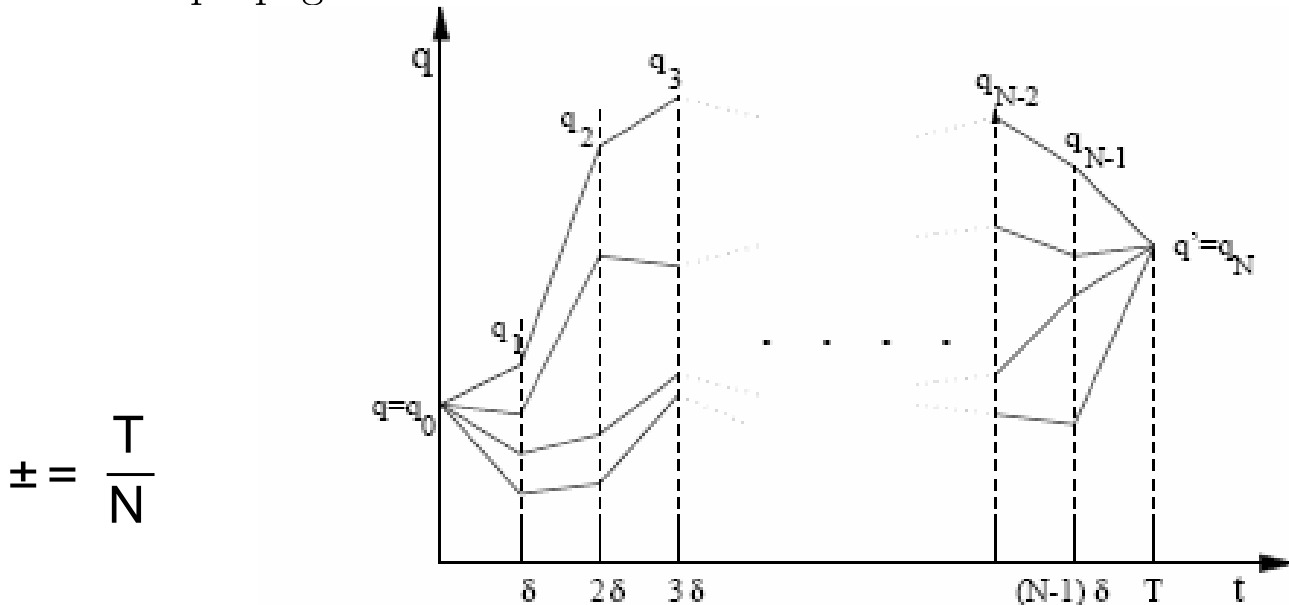
$$K(\mathbf{q}''t''; \mathbf{q}'t') = \int D[\mathbf{q}(t)] \exp \left[i \frac{S[\mathbf{q}(t)]}{\hbar} \right] = \lim_{N \rightarrow \infty} K^{[N]}(\mathbf{q}''t''; \mathbf{q}'t')$$

$$K^{[N]}(\mathbf{q}''t''; \mathbf{q}'t') = \int_{-\infty}^{\infty} \prod_{n=1}^{N-1} \frac{d\mathbf{q}_n}{A_n^{[N]}} \exp \left[i \frac{S^{[N]}[\mathbf{q}_0 \cdots \mathbf{q}_N]}{\hbar} \right] ; A_n^{[N]} = \left(\frac{2\pi i \hbar T}{m N} \right)^{\frac{f}{2}}$$

where,

$$S^{[N]}[\mathbf{q}_0 \cdots \mathbf{q}_N] = \frac{T}{N} \sum_{n=1}^N \left[\frac{m}{2} \frac{|\mathbf{q}_n - \mathbf{q}_{n-1}|^2}{(T/N)^2} - V \left((\mathbf{q}_{n-1} + \mathbf{q}_n)/2 \right) \right] ; \mathbf{q}_0 = \mathbf{q}' , \mathbf{q}_N = \mathbf{q}''$$

The $A_n^{[N]}$ are fixed so that for $V = 0$ one recovers the explicitly known expression for the free propagator.



The semi-classical approximation consists of evaluating the path integral in the **Saddle Point Approximation (SPA)**.

The SPA provides an expression for

$$I(\hbar) \doteq \int_{-\infty}^{\infty} e^{i \frac{f(x)}{\hbar}} dx$$

to leading order in \hbar when $\hbar \rightarrow 0$

If $f(x)$ has a single real stationary point $f'(x_0) = 0$, write $f(x) = f(x_0) + \frac{1}{2} f''(x_0)(x - x_0)^2$ and approximate:

$$\begin{aligned} I(\hbar) &\approx e^{i \frac{f(x_0)}{\hbar}} \int_{-\infty}^{\infty} e^{i \frac{f''(x_0)(x-x_0)^2}{2\hbar}} dx = e^{i \frac{f(x_0)}{\hbar}} \left(\frac{2\pi i \hbar}{f''(x_0)} \right)^{\frac{1}{2}} \\ &= e^{i \frac{f(x_0)}{\hbar} - i \frac{\pi}{2} \nu} \left(\frac{2\pi i \hbar}{|f''(x_0)|} \right)^{\frac{1}{2}} \end{aligned}$$

where $\nu = 1(0)$ when ($f''(x_0)$ is negative (positive)).

When there are several stationary points and if they are well separated, $I(\hbar)$ is the sum of their contributions.

For more details see e.g., Morse and Feshbach p437.

Back to the propagator and the path integral

$$K(\mathbf{q}''t''; \mathbf{q}'t') = \int D[\mathbf{q}(t)] \exp \left[i \frac{S[\mathbf{q}(t)]}{\hbar} \right].$$

$\mathbf{q}(t)$ a piecewise \mathcal{C}^1 path in config. space from \mathbf{q}' at t' to \mathbf{q}'' at t'' :
 $\mathbf{q}(t') = \mathbf{q}'$ and $\mathbf{q}(t'') = \mathbf{q}''$.

$S[\mathbf{q}(t)]$ the action functional: $S[\mathbf{q}(t)] = \int_{t'}^{t''} dt L(\mathbf{q}(t), \dot{\mathbf{q}}(t); t)$.

The Scl.Approx. is the leading term in the limit $\hbar \rightarrow 0$. The main contribution comes from the vicinity of the paths where the phase is stationary: $\delta S[\mathbf{q}(t)] = 0$ with the restriction: $\delta \mathbf{q}(t') = \delta \mathbf{q}(t'') = 0$.

$$\begin{aligned} \delta S[\mathbf{q}(t)] &= \int_{t'}^{t''} dt \left(\frac{\partial L[\mathbf{q}, \dot{\mathbf{q}}; t]}{\partial \mathbf{q}} \cdot \delta \mathbf{q} + \frac{\partial L[\mathbf{q}, \dot{\mathbf{q}}; t]}{\partial \dot{\mathbf{q}}} \cdot \delta \dot{\mathbf{q}} \right) \\ &= \int_{t'}^{t''} dt \left(\frac{\partial L[\mathbf{q}, \dot{\mathbf{q}}; t]}{\partial \mathbf{q}} - \frac{d}{dt} \frac{\partial L[\mathbf{q}, \dot{\mathbf{q}}; t]}{\partial \dot{\mathbf{q}}} \right) \cdot \delta \mathbf{q} + \left[\frac{\partial L[\mathbf{q}, \dot{\mathbf{q}}; t]}{\partial \dot{\mathbf{q}}} \cdot \delta \mathbf{q} \right]_{t'}^{t''} \\ &= - \int_{t'}^{t''} dt \left(\frac{\partial V[\mathbf{q}; t]}{\partial \mathbf{q}} + \frac{d}{dt} m \dot{\mathbf{q}} \right) \cdot \delta \mathbf{q} + [m \dot{\mathbf{q}} \cdot \delta \mathbf{q}]_{t'}^{t''} = 0 . \end{aligned}$$

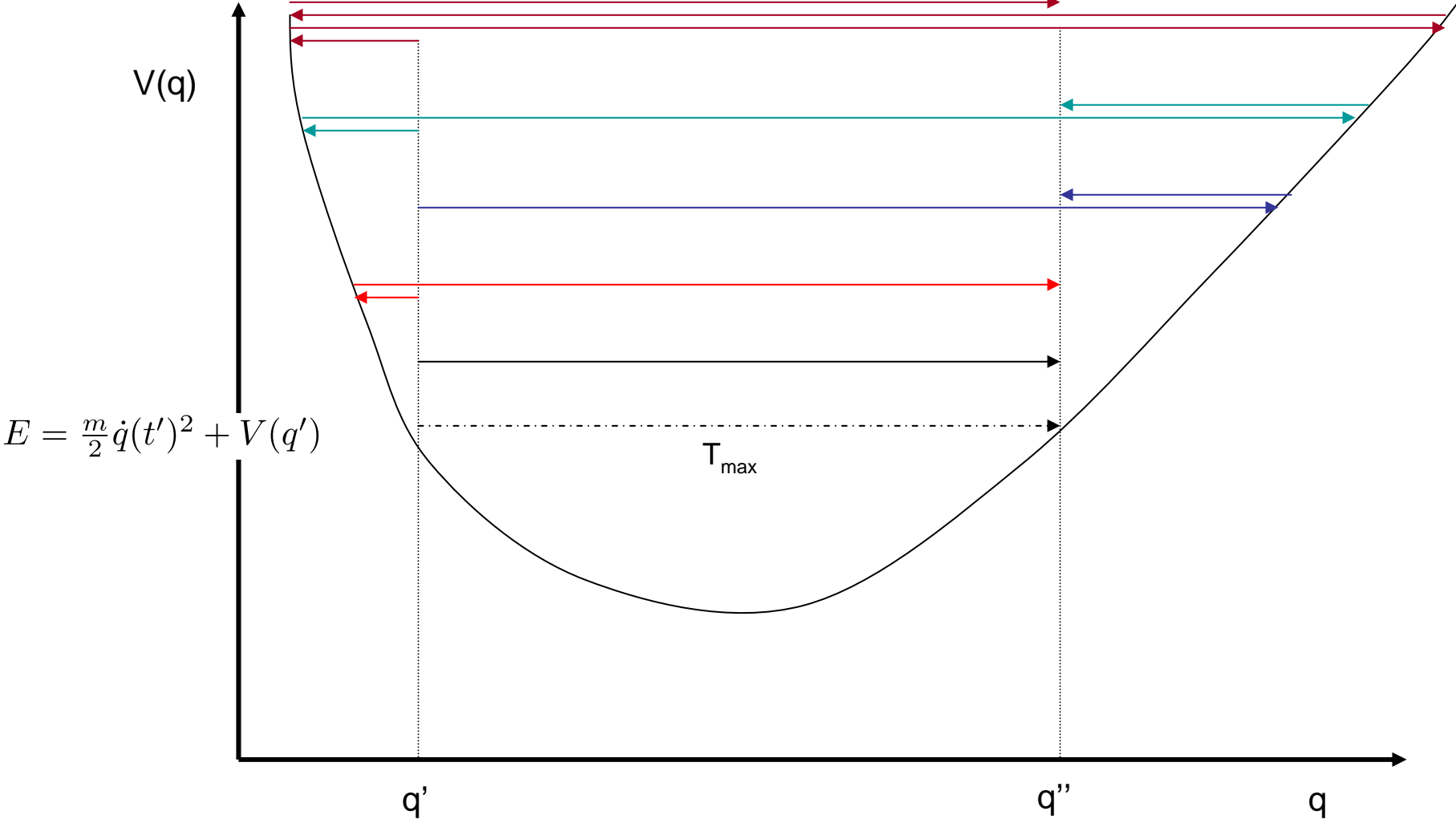
The saddle-point path is the **classical trajectory** which satisfies the Euler-Lagrange equation (Newton's second law):

$$\frac{\partial L[\mathbf{q}, \dot{\mathbf{q}}; t]}{\partial \mathbf{q}} - \frac{d}{dt} \frac{\partial L[\mathbf{q}_{cl}, \dot{\mathbf{q}}_{cl}; t]}{\partial \dot{\mathbf{q}}_{cl}} = 0 \quad \rightarrow \quad \frac{\partial V(\mathbf{q}_{cl})}{\partial \mathbf{q}_{cl}} + m \ddot{\mathbf{q}}_{cl} = 0$$

subject to the **boundary conditions**: $\mathbf{q}_{cl}(t') = \mathbf{q}'$, $\mathbf{q}_{cl}(t'') = \mathbf{q}''$.

Note: The boundary conditions do not determine a classical path uniquely! (examples below) However, there is no conflict with the uncertainty principle: the path is not prescribed by the simultaneous values of the position and the momentum.

Example: Several trajectories which satisfy the same boundary conditions.



T_{\max} : If $t'' - t' > T_{\max}$ direct transition becomes classically forbidden

Some properties of classical trajectories

i. Phase space *vs* configuration space: $\mathbf{p} \doteq \frac{\partial L(\mathbf{q}, \dot{\mathbf{q}}, t)}{\partial \dot{\mathbf{q}}} = m\dot{\mathbf{q}}$

ii. The classical trajectory is **uniquely** defined in terms of $2 \times f$ **initial** conditions at t' : $\mathbf{q}_{cl}(t') = \mathbf{q}'$, $\mathbf{p}_{cl}(t') = \mathbf{p}'$ or similarly by **final** conditions at t'' . We define it here in terms of $2 \times f$ **boundary** values $\mathbf{q}_{cl}(t') = \mathbf{q}'$, $\mathbf{q}_{cl}(t'') = \mathbf{q}''$. They do not guarantee existence or uniqueness.

iii. The classical action is a **function** of the boundary (or initial) conditions which define the classical trajectory.

$$\begin{aligned} \frac{\partial S_{cl}(\mathbf{q}', \mathbf{q}'')}{\partial \mathbf{q}'} &= \int_{t'}^{t''} dt \left(\frac{\partial L[\mathbf{q}_{cl}, \dot{\mathbf{q}}_{cl}; t]}{\partial \mathbf{q}_{cl}} \cdot \frac{\partial \mathbf{q}_{cl}}{\partial \mathbf{q}'} + \frac{\partial L[\mathbf{q}_{cl}, \dot{\mathbf{q}}_{cl}; t]}{\partial \dot{\mathbf{q}}_{cl}} \cdot \frac{\partial \dot{\mathbf{q}}_{cl}}{\partial \mathbf{q}'} \right) \\ &= \int_{t'}^{t''} dt \left(\frac{\partial L[\mathbf{q}, \dot{\mathbf{q}}; t]}{\partial \mathbf{q}} - \frac{d}{dt} \frac{\partial L[\mathbf{q}, \dot{\mathbf{q}}; t]}{\partial \dot{\mathbf{q}}} \right)_{cl} \cdot \frac{\partial \mathbf{q}_{cl}(t)}{\partial \mathbf{q}'} + \left[\frac{\partial L[\mathbf{q}_{cl}, \dot{\mathbf{q}}_{cl}; t]}{\partial \dot{\mathbf{q}}} \cdot \frac{\partial \mathbf{q}_{cl}(t)}{\partial \mathbf{q}'} \right]_{t'}^{t''} \\ &= \mathbf{p}_{cl}(t'') \frac{\partial \mathbf{q}_{cl}(t'')}{\partial \mathbf{q}'} - \mathbf{p}_{cl}(t') \frac{\partial \mathbf{q}_{cl}(t')}{\partial \mathbf{q}'} = -\mathbf{p}_{cl}(t') = -\mathbf{p}' . \end{aligned}$$

Similarly

$$\frac{\partial S_{cl}(\mathbf{q}', \mathbf{q}'')}{\partial \mathbf{q}''} = \mathbf{p}_{cl}(t'') \frac{\partial \mathbf{q}_{cl}(t'')}{\partial \mathbf{q}''} - \mathbf{p}_{cl}(t') \frac{\partial \mathbf{q}_{cl}(t')}{\partial \mathbf{q}''} = \mathbf{p}_{cl}(t'') = \mathbf{p}'' .$$

iv. The above is a proof that the classical dynamics can be thought of as a canonical transformation with the action $S_{cl}(\mathbf{q}', \mathbf{q}'')$ as the generating function.

Now that we have identified the classical trajectory (trajectories) as the saddle points we should compute the pre-exponential factor in the SPA for the path-integral. An elegant way to do this is offered if the path integral is defined in a different way.

The path expansion representation of the path integral

The path expansion method: $\mathbf{q}(t) = \xi(t) + \sum_{n=1}^{\infty} a_n \mathbf{u}_n(t)$

- $\xi(t)$: A reference path with $\xi(t') = \mathbf{q}'$; $\xi(t'') = \mathbf{q}''$

- $\{\mathbf{u}_n(t)\}_{n=1}^{\infty}$: A complete orthonormal basis

$$\int_{t'}^{t''} dt (\mathbf{u}_n(t) \cdot \mathbf{u}_m(t)) = \delta_{n,m} \text{ and } \mathbf{u}_n(t') = \mathbf{u}_n(t'') = 0 \forall n \in N$$

- $\{a_n\}_{n=1}^{\infty}$: path expansion coefficients $a_n \in R$

The N'th approximant to the path integral:

$$\mathbf{q}^{[N]}(t) = \xi(t) + \sum_{n=1}^N a_n \mathbf{u}_n(t) ; \rightarrow S[\mathbf{q}^{[N]}(t)] = S^{[N]}(\xi; a_1, \dots, a_N)$$

$$K^{[N]}(\mathbf{q}''t''; \mathbf{q}'t') = \left(\frac{m}{2\pi i \hbar (t'' - t')} \right)^{\frac{f}{2}} \int \dots \int \prod_{n=1}^N \frac{da_n}{A_n} \exp \left[i \frac{S^{[N]}(\xi; a_1, \dots, a_N)}{\hbar} \right] .$$

$$\text{For } f = 1 : A_n = \left(\frac{2\pi i \hbar (t'' - t')^2}{m(\pi n)^2} \right)^{\frac{1}{2}}$$

$$\text{In general : } n = f(k - 1) + j , 1 \leq j \leq f ; A_n = \left(\frac{2\pi i \hbar (t'' - t')^2}{m(\pi k)^2} \right)^{\frac{1}{2}}$$

$$K(\mathbf{q}''t''; \mathbf{q}'t') = \int D[\mathbf{q}(t)] \exp \left[i \frac{S[\mathbf{q}(t)]}{\hbar} \right] = \lim_{N \rightarrow \infty} K^{[N]}(\mathbf{q}''t''; \mathbf{q}'t')$$

Exercise 2:

a. Prove that the path expansion representation for K is independent of the choice of the reference path.

b. Consider $f = 1$. Choose $\xi(t) = \frac{q''-q'}{t''-t'}(t-t')+q'$ and $u_n(t) = \sqrt{\frac{2}{(t''-t')}} \sin \frac{\pi n(t-t')}{t''-t'}$.

Prove by direct integration that the path expansion expression for a free particle coincides with the exact expression given in a previous page.

The Semi-classical Approximation.

To use the path expansion method, we have to choose:

1. The reference path.
2. The orthonormal basis for the expansion.

The natural choice for the reference path is the classical path, being the path about which the action is stationary.

$$\xi(t) = \mathbf{q}_{cl}(t) \Leftrightarrow \delta S[\mathbf{q}_{cl}(t)] = 0. \quad ; \quad \mathbf{q}_{cl}(t') = \mathbf{q}' , \quad \mathbf{q}_{cl}(t'') = \mathbf{q}''$$

Expanding: $S[q_{cl} + \delta q(t)] = S[q_{cl}] + \frac{1}{2}\delta^2 S + \dots$, the expansion basis will be chosen to simplify $\delta^2 S$.

$$\delta S[\mathbf{q}(t)] = - \int_{t'}^{t''} dt \left(\frac{\partial V[\mathbf{q}; t]}{\partial \mathbf{q}} + \frac{d}{dt} m \dot{\mathbf{q}} \right) \cdot \delta \mathbf{q}$$

$$\delta^2 S = - \int_{t'}^{t''} dt \left(\frac{\partial^2 V(\mathbf{q}_{cl}(t); t)}{\partial \mathbf{q}^2} \delta \mathbf{q}(t) + m \frac{d}{dt} \delta \dot{\mathbf{q}} \right) \cdot \delta \mathbf{q}(t)$$

$$= - \int_{t'}^{t''} dt \delta \mathbf{q}(t) \left(V''(\mathbf{q}_{cl}(t); t) + m \frac{d^2}{dt^2} \right) \cdot \delta \mathbf{q}(t)$$

$$[V''(\mathbf{q}_{cl}(t); t)]_{i,j} = \left. \frac{\partial^2 V(\mathbf{q}, t)}{\partial q_i \partial q_j} \right|_{\mathbf{q}=\mathbf{q}_{cl}(t)} \quad ; \quad 1 \leq i, j \leq f$$

The operator

$$\Lambda(t) \doteq -m \frac{d^2}{dt^2} - V''(\mathbf{q}_{cl}(t); t) \quad ; \quad t \in [t', t'']$$

plays an essential rôle in the following, and it deserves a proper introduction.

Stability of classical orbits.

A classical trajectory $\mathbf{q}_{cl}(t)$ is a solution of the equation of motion:

$$m\ddot{\mathbf{q}} + \frac{\partial V(\mathbf{q})}{\partial \mathbf{q}} = 0$$

Subject to the *initial* conditions at t' , namely $\mathbf{q}_{cl}(t') = \mathbf{q}_{in}$ and $\dot{\mathbf{q}}_{cl}(t') = \dot{\mathbf{q}}_{in}$.

A near-by trajectory satisfies:

$$m(\ddot{\mathbf{q}}_{cl} + \delta\ddot{\mathbf{q}}) + \frac{\partial V(\mathbf{q}_{cl} + \delta\mathbf{q}; t)}{\partial \mathbf{q}} = 0$$

to 1st order :

$$m\delta\ddot{\mathbf{q}} + V''(\mathbf{q}_{cl}(t); t) \delta\mathbf{q} = \Lambda(t) \delta\mathbf{q} = 0.$$

The sensitivity of the trajectory to small changes in the initial j 'th position: $\mathbf{y}^{(j)}(t) \doteq \partial\mathbf{q}(t)/\partial q_j(t')$ is a solution of the stability equation subject to the initial condition $y_k^{(j)}(t') = \delta_{jk}$; $\dot{\mathbf{y}}(t') = 0$. Similarly, the sensitivity of the trajectory to small changes in the initial j 'th velocity: $\mathbf{z}^{(j)}(t) \doteq \partial\mathbf{q}(t)/\partial \dot{q}_j(t')$ is a solution of the stability equation subject to the initial condition $\dot{z}_k^{(j)}(t') = \delta_{jk}$; $\mathbf{z}^{(j)}(t') = 0$. The combined set of $2f$ independent solutions of the stability equation provide all the information about the (linear) stability of the trajectory. The solutions are some times referred to as the “Jacobi fields”.

It is convenient to generalize slightly the definition of the stability operator (and change its sign):

$$\Lambda(t; \alpha) \doteq -m \frac{d^2}{dt^2} - \alpha V''(\mathbf{q}_{cl}(t); t) \quad ; \quad t \in [t', t'']$$

(α interpolates between free motion ($\alpha = 0$) and the problem of interest ($\alpha = 1$)).

Some properties of $\Lambda(t; \alpha)$:

i. $\Lambda(t; \alpha)$ is of Sturm -Liouville (Schrödinger) type. Its eigenfunctions define a natural orthonormal basis, inherent to the problem at hand:

$\Lambda(t; \alpha) \mathbf{u}_n(t; \alpha) = \lambda_n(\alpha) \mathbf{u}_n(t; \alpha)$ with boundary conditions $\mathbf{u}_n(t') = \mathbf{u}_n(t'') = 0$.

ii. Wronskian relation: Let $\mathbf{y}^{(1)}$ and $\mathbf{y}^{(2)}$ be two solutions of the stability equation. Then,

$$\mathbf{y}^{(1)} \cdot \dot{\mathbf{y}}^{(2)} - \dot{\mathbf{y}}^{(1)} \cdot \mathbf{y}^{(2)} = \text{const} .$$

iii. Free motion:

$$\Lambda_{i,j}(t; \alpha = 0) = \delta_{i,j} m \frac{d^2}{dt^2} \quad \text{with} \quad \leq i, j \leq f .$$

Denote by $\mathbf{e}^{(j)}$ the f dimensional unit vector pointing at the j direction. $n = f(k-1) + j$

$$\mathbf{u}_n(t, \alpha = 0) = \mathbf{e}^{(j)} \sqrt{\frac{2}{(t'' - t')}} \sin \pi k \frac{t - t'}{t'' - t'} \quad ; \quad \lambda_n(\alpha = 0) = m \left(\frac{\pi k}{t'' - t'} \right)^2 .$$

The Jacobi fields for the free motion are

$$\mathbf{y}^{(j)}(t) = (t - t') \cdot \mathbf{e}^{(j)} \quad ; \quad \mathbf{z}^{(j)}(t) = \mathbf{e}^{(j)} .$$

iv. As long as $V''(\mathbf{q}_{cl}(t); t)$ is finite in the interval $[t', t'']$,

$$\text{For } n \rightarrow \infty : (\lambda_n(\alpha) - \lambda_n(0)) \rightarrow \text{const}$$

v. Only a finite number of the $\lambda_n(\alpha)$ are negative. For any α the spectrum become positive if the time interval $[t', t'']$ is sufficiently small.

Exercise 3:

- a. Consider the perturbation of a classical trajectory induced by a small variation in the potential, and show that it satisfies an inhomogeneous equation of the type $\Lambda \mathbf{y} = \mathbf{w}(t)$.
- b. For simplicity assume $f=1$. Express the perturbation of the trajectory in terms of the independent solutions of the homogeneous stability equation. (To get bonus points: generalize to any f).

Back to the evolution operator:

Using the eigenfunctions $\mathbf{u}_n(t, 1)$ as a basis, $\mathbf{q}(t) = \mathbf{q}_{cl}(t) + \sum_{n=1}^{\infty} a_n \mathbf{u}_n(t; 1)$.

$$S[q(t); a_1, a_2, \dots] \approx S[\mathbf{q}_{cl}] + \frac{1}{2} \sum_{n=1}^{\infty} \lambda_n(1) a_n^2 . \rightarrow \text{an immense simplification!}$$

$$K(\mathbf{q}''t''; \mathbf{q}'t') = \left(\frac{m}{2\pi i \hbar (t'' - t')} \right)^{\frac{f}{2}} \int \dots \int \prod_{n=1}^{\infty} \frac{da_n}{A_n} \exp \left[i \frac{S(\xi; a_1, a_2, \dots)}{\hbar} \right]$$

$$\approx \left(\frac{m}{2\pi i \hbar (t'' - t')} \right)^{\frac{f}{2}} \exp \left[i \frac{S[\mathbf{q}_{cl}]}{\hbar} \right] \prod_{n=1}^{\infty} \int_{-\infty}^{\infty} \exp \left[\frac{i}{2\hbar} \lambda_n(1) a_n^2 \right] \frac{da_n}{A_n}$$

$$= \left(\frac{m}{2\pi i \hbar (t'' - t')} \right)^{\frac{f}{2}} \exp \left[i \frac{S[\mathbf{q}_{cl}]}{\hbar} \right] \prod_{n=1}^{\infty} \left(\frac{2\pi \hbar}{|\lambda_n(1)|} \right)^{\frac{1}{2}} e^{i \frac{\pi}{4} \text{sgn}(\lambda_n)} / A_n$$

$$\text{finally : } K_{scl}(\mathbf{q}''t''; \mathbf{q}'t') = \left(\frac{m}{2\pi i \hbar (t'' - t')} \right)^{\frac{f}{2}} \exp \left[i \frac{S[\mathbf{q}_{cl}]}{\hbar} \right] e^{i \frac{\pi}{2} \nu} \prod_{n=1}^{\infty} \left(\frac{\lambda_n(0)}{|\lambda_n(1)|} \right)^{\frac{1}{2}}$$

ν is the number of negative $\lambda_n(1)$. This is the Maslov index of the classical trajectory. Because of *iv.* above the infinite product converges. Its value can be derived from the following theorem:

Theorem (Levit, Smilansky)

Let $\mathbf{y}^{(j)}(t, \alpha)$ be the Jacobi fields: $\Lambda(t; \alpha)\mathbf{y}^{(j)}(t; \alpha) = 0$,
subject to the initial conditions $\mathbf{y}^{(j)}(t'; \alpha) = 0$; $\dot{\mathbf{y}}^{(j)}(t'; \alpha) = \mathbf{e}^{(j)}$.

Then:

1. $\prod_{n=1}^{\infty} \frac{\lambda_n(0)}{\lambda_n(1)} = \frac{\det[y_l^{(j)}(t''; 0)]}{\det[y_l^{(j)}(t''; 1)]}$
2. $\nu =$ the number of times $\det[y_l^{(j)}(t; 1)]$ changes its sign in (t', t'') .

We can now collect all the results prepared above, (and remember that the momentum \mathbf{p} conjugate to \mathbf{q} is just $\mathbf{p} = m\dot{\mathbf{q}}$) to get the final expression for the semiclassical propagator:

$$K_{scl}(\mathbf{q}''t''; \mathbf{q}'t') = \left(\frac{1}{2\pi i\hbar} \right)^{\frac{f}{2}} \sum_{cl} \frac{\exp i \left(\frac{S_{cl}}{\hbar} - \frac{\pi}{2} \nu_{cl} \right)}{\left| \det \frac{\partial q_j(t'')}{\partial p_k(t')} \right|_{cl}^{\frac{1}{2}}}$$

The summation is over all the classical trajectories which satisfy the boundary conditions $\mathbf{q}(t') = \mathbf{q}'$; $\mathbf{q}(t'') = \mathbf{q}''$). This expression was first derived by Van Vleck, and we shall dedicate the rest of this lecture to interpret and explain it.

Classical bones: dynamics (trajectory), action, stability

Quantum flesh : transition amplitude, interference, the quantum scale: \sim

Comments and interpretation

i. The semi-classical transition probability.

$|K(\mathbf{q}''t''; \mathbf{q}'t')|^2$ is the probability to make a transition from the quantum state localized at \mathbf{q}' to a state localized at \mathbf{q}'' at the time $(t'' - t')$. Classically, the transition determines a certain value of the initial momentum \mathbf{p}' . Denote by $\delta q'_j, \delta p'_j$ the position and momentum uncertainties of an initial state centered at the initial phase space point. It is assumed that the $\delta q'_j$ are small so the initial state is well localized. Note: a quantum state occupies a phase space of volume $vol(\delta q)vol(\delta p) = (2\pi\hbar)^f$. The classical dynamics maps the initial $2f$ dimensional parallelepiped to another parallelepiped centered at the final phase space point $\mathbf{q}'', \mathbf{p}''$. The probability to start in a volume differential $d^f q'$ about \mathbf{q}' and end in a volume differential $d^f q''$ about \mathbf{q}'' is

$$P(\mathbf{q}''t''; \mathbf{q}'t')d^f q'd^f q'' = \frac{d^f q'}{vol(\delta q')} \frac{d^f q''}{vol(\delta q'')} .$$

However,

$$vol(\delta q'') = \left| \det \frac{\partial q_j(t'')}{\partial p_k(t')} \right|_{cl} vol(\delta p') .$$

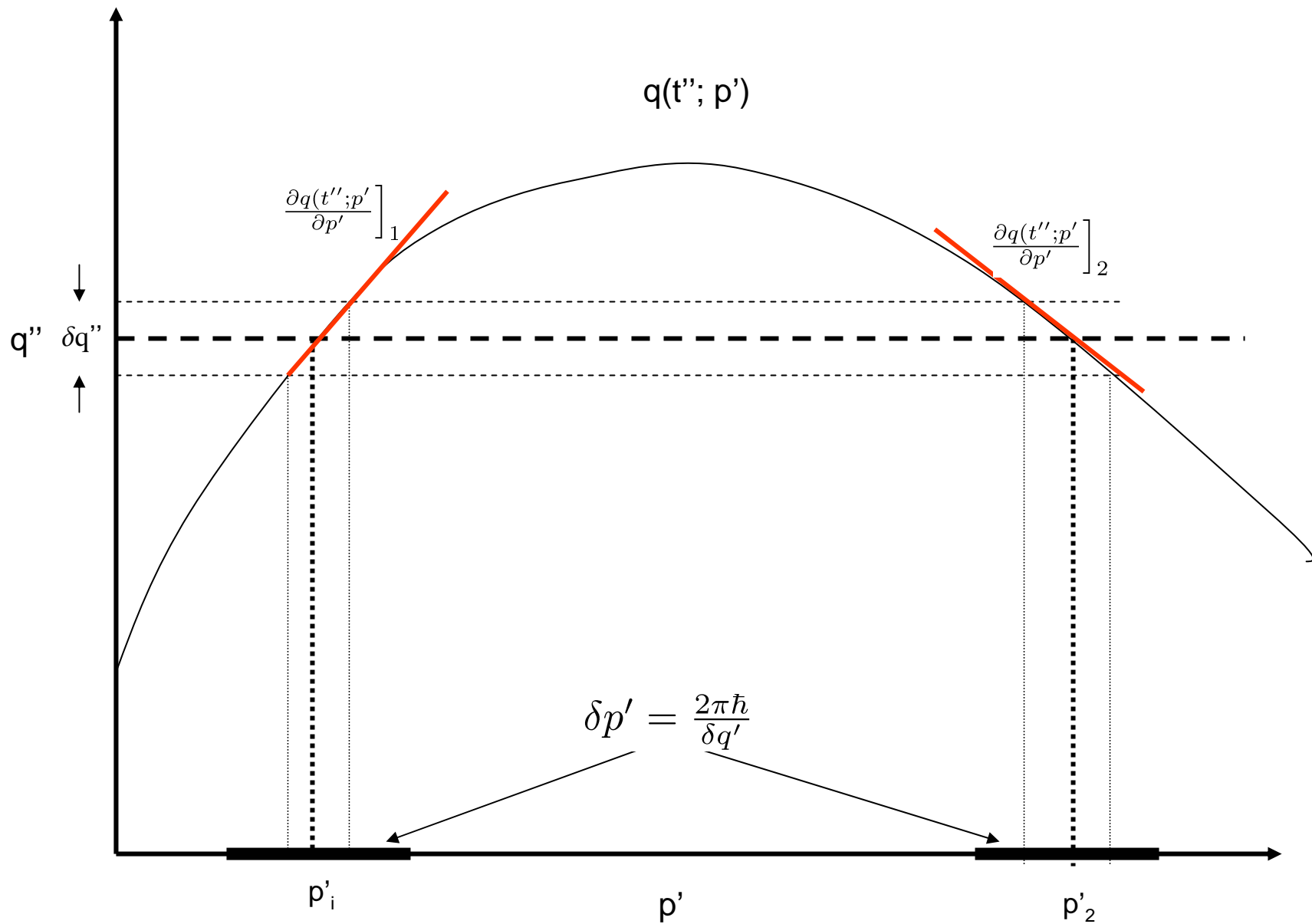
Thus,

$$P_{cl}(\mathbf{q}''t''; \mathbf{q}'t') = (2\pi\hbar)^{-f} \left| \det \frac{\partial q_j(t'')}{\partial p_k(t')} \right|_{cl}^{-1} .$$

$$|K_{scl}(\mathbf{q}''t''; \mathbf{q}'t')|^2 = \sum_{cl} P_{cl}(\mathbf{q}''t''; \mathbf{q}'t') + 2 \sum_{cl \neq \bar{cl}} |P_{cl}P_{\bar{cl}}|^{\frac{1}{2}} \cos\left(\frac{\Delta S}{\hbar} - \frac{\pi}{2}\Delta\nu\right)$$

In the limit $\hbar \rightarrow 0$ the interference terms vanish (in the weak sense).

Classical transition probability



ii. Unitarity of the semi-classical evolution operator. (f=1 for simplicity)

To be consistent: all integrals must be performed in the SPA.

$$I(q'', \bar{q}'') \doteq \int dq' K_{scl}(q''t''; q't') K_{scl}^*(\bar{q}''t''; q't') = \frac{1}{2\pi\hbar} \int dq' \frac{e^{\left[\frac{i}{\hbar}(S_{cl}(q'', q') - S_{cl}(\bar{q}'', q')) - \frac{i\pi}{2}(\nu - \bar{\nu})\right]}}{\left| \frac{\partial q(t'')}{\partial p(t')} \frac{\partial \bar{q}(t'')}{\partial p(t')} \right|^{\frac{1}{2}}}.$$

Saddle point condition: $\frac{\partial S_{cl}(q'', q')}{\partial q'} = \frac{\partial S_{cl}(\bar{q}'', q')}{\partial q'}$ hence: $p'(q'') = p'(\bar{q}'')$, implying the trajectories coincide and $q'' = \bar{q}''$. Since most of the contribution is in the neighborhood $q'' \approx \bar{q}''$ write for the action difference in the exponent $\frac{\partial S_{cl}}{\partial q''}(q'' - \bar{q}'')$.

$$I(q'', \bar{q}'') \approx \frac{1}{2\pi\hbar} \int dq' \frac{e^{\frac{i}{\hbar} \frac{\partial S_{cl}}{\partial q''}(q'' - \bar{q}'')}}{\left| \frac{\partial q(t'')}{\partial p(t')} \right|}.$$

$$\frac{1}{\frac{\partial q''}{\partial p'}} = -\frac{\partial^2 S_{cl}(q', q'')}{\partial q' \partial q''} = -\frac{\partial p''}{\partial q'} \rightarrow I(q'', \bar{q}'') \approx \frac{1}{2\pi\hbar} \int dp'' e^{\frac{i}{\hbar} p''(q'' - \bar{q}'')} = \delta(q'' - \bar{q}'').$$

iii. The semi classical propagator has the semi-group property (Composition), if the intermediate integration is carried out by the SPA. The proof is left as an exercise.

Exercise 4:(Difficult)

Prove that the semi-classical propagator satisfies (semi-classically) the composition rule. Prove by performing the integral over the intermediate coordinate by the SPA)

iv. Focal points are the points where $\det \left. \frac{\partial q_j(t'')}{\partial p_k(t')} \right|_{cl} = 0$. At focal points, classical trajectories which satisfy the same boundary conditions coalesce.

The semi-classical approximation diverges at such points. The loci of focal points are the *caustics* (From Greek "kaustos" = burnt). The quantum transition probability is enhanced but does not diverge at caustics. One has to use a uniform semi-classical theory to describe the phenomenon - this goes beyond the present course.

Example A particle in an inverse square potential :

$$L(x, \dot{x}) = \frac{1}{2}(\dot{x}^2 - \frac{l^2}{x^2}) \rightarrow \ddot{x} = -\frac{l^2}{x^3}$$

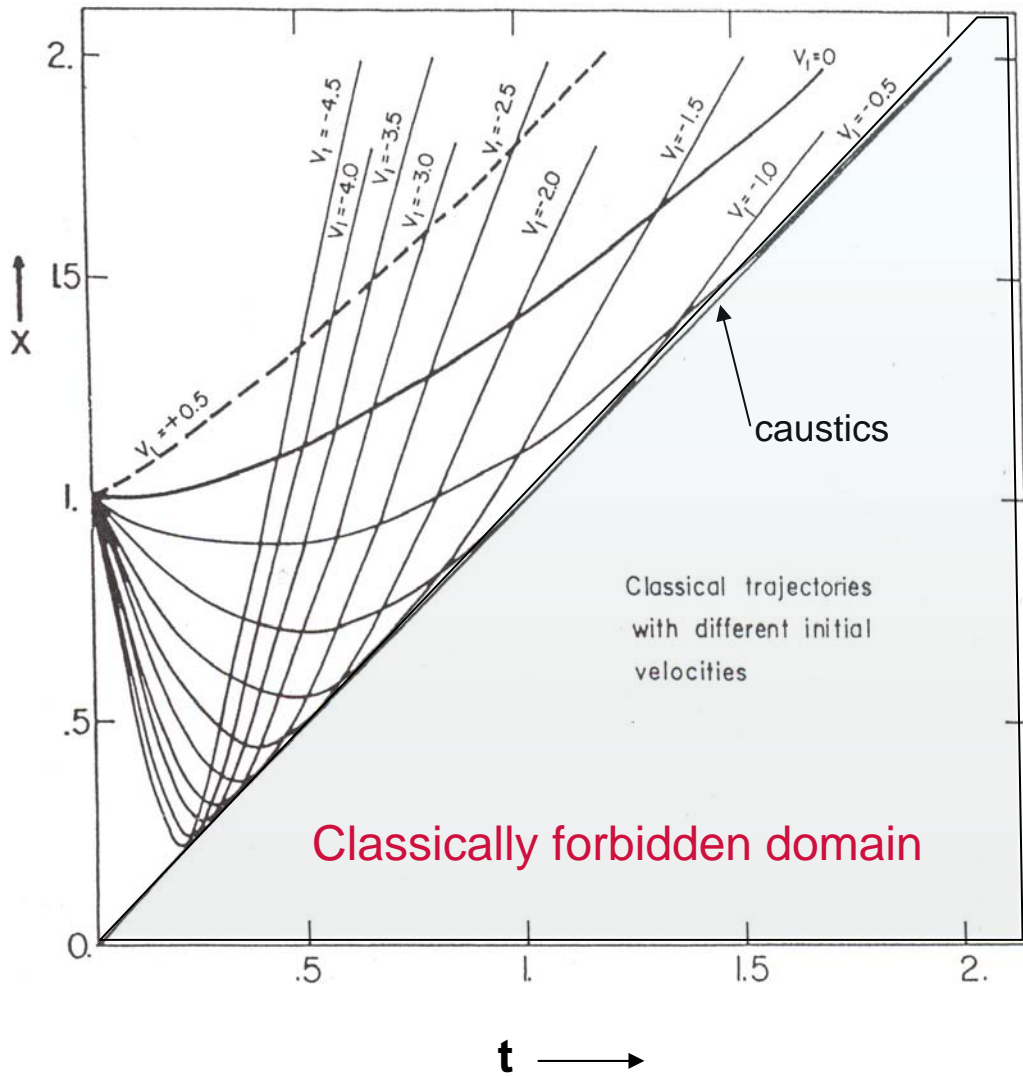
The trajectory: $(x_{cl}(t; x', \dot{x}'))^2 = (t \dot{x}' + x')^2 + t^2 \left(\frac{l}{x'}\right)^2$; ($t' = 0$).

The **initial conditions** uniquely define a classical trajectory.

The **boundary conditions** can be satisfied by either two trajectories or none:

$$\dot{x}' = \frac{1}{t} \left(-x' \pm \sqrt{x'^2 - t^2 \left(\frac{l}{x'}\right)^2} \right) .$$

Caustics : $\frac{\partial x(t; \dot{x}')}{\partial \dot{x}'} = 0$ hence $\dot{x}' = -\frac{x'}{t}$ and therefore $x'' = t \frac{l}{x'}$.



Example: The evolution operator for the harmonic oscillator

$$L = \frac{m}{2} (\dot{q}^2 - \omega^2 q^2)$$

Class. traj. (determined uniquely by **bound conditions** except at $T = \frac{\pi}{\omega}n$):

$$q_{cl}(q'', q'; T) = q' \cos \omega t + \frac{q'' - q' \cos \omega T}{\sin \omega T} \sin \omega t$$

$$\dot{q}_{cl}(q'', q'; T) = \omega \left[-q' \sin \omega t + \frac{q'' - q' \cos \omega T}{\sin \omega T} \cos \omega t \right]$$

$$S_{cl}(q'', q'; T) = \frac{m\omega}{2 \sin \omega T} [\cos \omega T (q''^2 + q'^2) - 2q'q'']$$

Class. traj. (determined uniquely by the **initial conditions** except at $T = \frac{\pi}{\omega}n$):

$$q_{cl}(q', \dot{q}'; T) = q' \cos \omega t + \dot{q}' \frac{\sin \omega t}{\omega}$$

The stability operator

$$\Lambda = m \left(-\frac{d^2}{dt^2} - \omega^2 \right) ; \text{ Spectrum } \lambda_n = m \left(\left(\frac{\pi n}{T} \right)^2 - \omega^2 \right)$$

$$\prod_n \frac{\lambda_n(\omega = 0)}{\lambda_n(\omega)} = \prod_n \left(1 - \left(\frac{\omega T}{\pi} \right)^2 \frac{1}{n^2} \right) = \frac{\sin \omega T}{\omega T} \text{ (last step due to Euler)}$$

$$y(t) = \frac{\sin \omega t}{\omega} ; y(t; \omega = 0) = t ; \text{ Caustics at } t = \frac{\pi}{\omega}n .$$

harmonic oscillator cont.

$$K_{scl}(q''T; q'0) = \frac{1}{2\pi i\hbar} \left(\frac{m\omega}{\sin \omega T} \right)^{\frac{1}{2}} \exp i \left[\frac{m\omega}{2\hbar \sin \omega T} (\cos \omega T (q''^2 + q'^2) - 2q'q'') \right]$$

Exercise 4:

- Discuss the Caustics in this system.
- Check in the text books that the semi classical approximation reconstructs the exact result. Explain why.
- Prove that

$$\lim_{\epsilon \rightarrow 0} K(q'', T = \frac{\pi}{\omega} n + \epsilon; q', 0) = \delta(q'' - (-1)^n q') .$$

End of section I

A THEOREM ON INFINITE PRODUCTS OF EIGENVALUES OF STURM-LIOUVILLE TYPE OPERATORS

S. LEVIT AND U. SMILANSKY

ABSTRACT. Infinite products of ratios of eigenvalues of Sturm-Liouville operators are expressed in a closed form in terms of corresponding solutions of initial-value problems.

Introduction. Gaussian path integrals are defined by

$$(1) \quad I = \int_{\text{paths}} D[\vec{\eta}(t)] \exp[iS[\vec{\eta}(t)]]$$

where

$$(2) \quad S[\vec{\eta}(t)] = \int_0^T (\vec{\eta}(t) \cdot \Lambda(t)\vec{\eta}(t)) dt,$$

and $\vec{\eta}(t)$ are the N dimensional paths satisfying the end conditions $\vec{\eta}(0) = \vec{\eta}(T) = 0$. $\Lambda(t)$ is a differential operator of second order in (d/dt) acting on the space of paths. Such path integrals are often encountered in physical problems, e.g. the formulation of quantum mechanics [1].

The integral (1) can be evaluated in terms of the infinite product of the eigenvalues of $\Lambda(t)$ [2], [3]. In this note we present a theorem which enables one to express these infinite products in a closed form.

The theorem will be presented with a detailed proof for the simple case of a one dimensional problem ($N = 1$). The extension to $N > 1$ will be formulated but a detailed proof will not be supplied since it follows the same lines as for $N = 1$.

THEOREM 1. Let the differential operator

$$(3) \quad \Lambda(\alpha; t) = (d/dt)(p(t)d/dt) + \alpha q(t)$$

be defined for $0 \leq t \leq T$, $0 \leq \alpha \leq 1$, where $p(t)$ and $q(t)$ are smooth functions of t , $p(t) > p_0 > 0$.

Let $\lambda_k(\alpha)$ and $U^{(k)}(\alpha; t)$ be the eigenvalues and eigenfunctions for the boundary-value problem

$$(4) \quad \Lambda(\alpha; t)U(\alpha; t) + \lambda(\alpha)U(\alpha; t) = 0, \quad U(\alpha; 0) = U(\alpha; T) = 0.$$

Let $y(\alpha; t)$ be the solution of the initial-value problem

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$$(5) \quad \Lambda(\alpha; t)y(\alpha; t) = 0, \quad y(\alpha; 0) = 0, \quad (d/dt)y(\alpha; 0) = 1.$$

Then, for every α

$$(6) \quad \left| \prod_{k=1}^{\infty} \frac{\lambda_k(\alpha)}{\lambda_k(0)} \right| = \left| \frac{y(\alpha; T)}{y(0; T)} \right|.$$

PROOF. The following points should be observed:

(a) For all k , $\lambda_k(0) > 0$ and for large k ,

$$\lambda_k(0) \cong \left[\pi / \int_0^T \frac{dt}{\sqrt{p(t)}} \right]^2 \cdot k^2, \quad [4].$$

(b) The functions $\lambda_k(\alpha)$, $U^{(k)}(\alpha; t)$ and $y(\alpha; t)$ are analytic in α [5].

(c) For large k , $|\lambda_k(\alpha) - \lambda_k(0)| \leq \alpha \cdot M$ [4] with M independent of α or k . Hence the product on the left-hand side of (6) converges uniformly for all finite values of α .

(d) There is a finite number of nonpositive eigenvalues for a given α [6]. Hence the product on the left-hand side of (6) vanishes only at a finite number of α values, in the interval $0 \leq \alpha \leq 1$.

A necessary and sufficient condition for $y(\alpha; T)$ to vanish is that one of the $\lambda_k(\alpha)$ vanishes. Hence the two sides of equation (6) vanish simultaneously.

Consider now the functions:

$$(7) \quad f(\alpha) = \prod_{k=1}^{\infty} \frac{\lambda_k(\alpha)}{\lambda_k(0)},$$

$$(8) \quad \tilde{f}(\alpha) = y(\alpha; T)/y(0; T).$$

Since by construction $f(0) = \tilde{f}(0) = 1$, the theorem will be proved once it is demonstrated that $(d/d\alpha)f(\alpha)/f(\alpha) = (d/d\alpha)\tilde{f}(\alpha)/\tilde{f}(\alpha)$, for all α satisfying $f(\alpha) \neq 0$.

By virtue of (c) one can differentiate the left-hand side of equation (7) as if it were a finite product and get

$$(9) \quad \frac{d}{d\alpha} f(\alpha)/f(\alpha) = \sum_{k=1}^{\infty} \frac{d\lambda_k(\alpha)}{d\alpha} \frac{1}{\lambda_k(\alpha)}.$$

It can easily be shown that

$$(10) \quad \frac{d\lambda_k(\alpha)}{d\alpha} = - \int_0^T [U^{(k)}(\alpha; t)]^2 q(t) dt,$$

where $U^{(k)}(\alpha; t)$ are the solutions of (4) subject to the normalization

$$(11) \quad \int_0^T [U^{(k)}(\alpha; t)]^2 dt = 1.$$

Since the integral in (10) is bounded by $\text{Max}|q(t)|$ and because of (c), the series on the right-hand side of (9) converges uniformly and the summation and integration operations could be interchanged to yield

$$(12) \quad \frac{d}{d\alpha} f(\alpha)/f(\alpha) = \int_0^T G_{\lambda=0}(t, t, \alpha)q(t) dt$$

with

$$(13) \quad G_{\lambda}(t, t', \alpha) = \sum_{k=1}^{\infty} \frac{U^{(k)}(\alpha; t)U^{(k)}(\alpha; t')}{\lambda - \lambda_k(\alpha)}, \quad // \rho \lambda$$

which is the spectral representation of Green's function for the boundary-value problem (4).

Returning to the initial value problem (5) and differentiating it with respect to α , one gets that $z(\alpha; t) \equiv dy(\alpha; t)/d\alpha$ is a solution of the initial-value problem

$$(14) \quad \Lambda(\alpha; t)z(\alpha; t) = -q(t)y(\alpha; t), \quad z(\alpha; 0) = 0, \quad (d/dt)z(\alpha; 0) = 0.$$

The solution of (14) is expressed in terms of the solution $y(\alpha; t)$ of (5) and the solution $\bar{y}(\alpha; t)$ of the adjoint problem

$$(15) \quad \Lambda(\alpha; t)\bar{y}(\alpha; t) = 0, \quad \bar{y}(\alpha; T) = 0, \quad (d/dt)\bar{y}(\alpha; T) = 1.$$

Applying the method of variation of the parameters, one can prove that the solution of (14) is given by

$$(16) \quad z(\alpha; t) = \left[y(\alpha; t) \int_0^t y(\alpha; t')\bar{y}(\alpha; t')q(t') dt' - \bar{y}(\alpha; t) \int_0^t y(\alpha; t')y(\alpha; t')q(t') dt' \right] / W,$$

where

$$(17) \quad W = p(t)[y d\bar{y}/dt - \bar{y} dy/dt] = \text{const.}$$

Hence

$$(18) \quad z(\alpha; T) = \frac{dy(\alpha; T)}{d\alpha} = y(\alpha; T) \int_0^T \bar{y}(\alpha; t)y(\alpha; t)q(t) dt / W \\ = y(\alpha; T) \int_0^T G_{\lambda=0}(t, t, \alpha)q(t) dt$$

where $G_{\lambda}(t, t', \alpha)$ is again Green's function for the boundary-value problem (4), expressed in terms of the solutions of the initial-value problem (5) and its adjoint (15). A comparison of (18) with (12) completes the proof.

We now turn to the generalization of Theorem 1 to the N dimensional case. The functions $p(t)$ and $q(t)$ of (3) are now replaced by the $N \times N$ symmetric matrices $P(t)$ and $Q(t)$. $P(t)$ is required to be positive definite for all $0 \leq t \leq T$. The N dimensional vectors on which $\Lambda(\alpha; t)$ acts are denoted by $\vec{U}(\alpha; t) \equiv (U_1(\alpha; t), \dots, U_N(\alpha; t))$.

THEOREM 2. *Let a differential operator*

$$(19) \quad \Lambda(\alpha; t) = (d/dt)(P(t)d/dt) + \alpha Q(t)$$

be defined for $0 \leq t \leq T$, $0 \leq \alpha \leq 1$, with $P(t)$ and $Q(t)$ as discussed above.

Let $\lambda_k(\alpha)$ and $\vec{U}^{(k)}(\alpha; t)$ be the eigenvalues and eigenfunctions for the boundary-value problem

$$(20) \quad \Lambda(\alpha; t)\vec{U}(\alpha; t) + \lambda(\alpha)\vec{U}(\alpha; t) = 0, \quad \vec{U}(\alpha; 0) = \vec{U}(\alpha; T) = 0.$$

Let $\vec{y}^{(j)}(\alpha; t)$ ($j = 1, \dots, N$) be the N independent solutions of the initial-value problem

$$(21) \quad \Lambda(\alpha; t)\vec{y}^{(j)}(\alpha; t) = 0, \quad \vec{y}^{(j)}(\alpha; 0) = 0, \quad (d/dt)y_i^{(j)}(\alpha; 0) = \delta_{ij}.$$

Let $D(\alpha)$ be

$$(22) \quad D(\alpha) = \det[y_i^{(j)}(\alpha; T)].$$

Then, for every α

$$(23) \quad \left| \prod_{k=1}^{\infty} \frac{\lambda_k(\alpha)}{\lambda_k(0)} \right| = \left| \frac{D(\alpha)}{D(0)} \right|.$$

OUTLINE OF THE PROOF. The proof of Theorem 2 is again based on evaluating the logarithmic derivative of the two sides of (23). Once again it is shown that the logarithmic derivative can be expanded in the form

$$(24) \quad \frac{df(\alpha)}{d\alpha} / f(\alpha) = \sum_{j,i=1}^N \int_0^T dt G_{j,i}^{(\lambda=0)}(t, t, \alpha)Q_{ij}(t) = \frac{d\tilde{f}(\alpha)}{d\alpha} / \tilde{f}(\alpha)$$

where $f(\alpha)$ and $\tilde{f}(\alpha)$ denote the functions of α on the left- and right-hand sides of equation (23) respectively. The Green's "function" is a matrix $G_{j,i}^{(\lambda)}(t, t', \alpha)$. In proving (24) use is made of the two equivalent methods to express the Green's function, the spectral representation and the representation by means of the $2N$ independent solutions of equation (21) and its adjoint.

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